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Appendix B

ANALYSIS OF EMISSION CONTROL BY A CATALYTIC RECUPERATOR AND BY UPSTREAM MONOLITHS

INTRODUCTION

[redacted] using post turbine catalytic monoliths and catalytically active exhaust-side recuperator surfaces to remove hydrocarbon and carbon monoxide emissions from the Capstone turbogenerators. [redacted] This report represents the detailed analysis, calculations, results, and conclusions. Also attached are the MathSoft Mathcad™ 6+ documents comprising the analyses and an Excel 5.0 spreadsheet of the findings.

TRANSPORT AND KINETIC ANALYSIS OF THE RECUPERATOR AND MONOLITHS

The analysis of the conversion of heptene (C_7H_{14}), methane (CH_4), and carbon monoxide (CO), were completed for several configurations of a recuperator and honeycomb catalytic converters. The method used was a MATHCAD program, and the procedures were similar to the document sent to Capstone [redacted] ~~(CAPSTONE.MCD.document)~~.

The analyses consist of the following features (see ~~printouts for CPSTONE5.MCD and CPSTONE6.MCD)~~:

Gas Properties

- The properties of the gases used in the combustion mixture are described on pages 1-8.
- The gas compositions both for complete combustion air with fuel equivalence ratio 0.1 in moist (2 vol% water vapor) air, as specified in the problem statement, and also for an adiabatic temperature rise from 1000° to 1511_F using heptene are defined on page 2. The difference in properties between these two compositions is insignificant.
- Essential transport properties, such as the diffusivities of the added gases are determined on pages 3-4.
- Mixture properties such as viscosity, thermal conductivity, heat capacity, and various dimensionless transport numbers such as the Prandtl and Schmidt numbers are defined and calculated on pages 5-8.

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B1

Recuperator and Converter Dimensions and Operating Conditions

- The dimensions of the honeycomb sizes from 100 to 800 cells/in.^{2} are defined on page 9 along with the size and dimensions of the recuperator and the upstream monolith converters.
- The five operating combustion conditions representing the different power level cases for the turbogenerator are specified on pages 9-10.
- The pressure drop for the 600 or 800 cells/in^2 recuperator is determined on page 11, and the analysis of heat transfer within the recuperator is described on page 12.

Recuperator Performance

- Mass transfer rates to the wall of the recuperator (assuming very fast conversion kinetics at the wall) are described on pages 13-14 for all three added components (C_7H_{14}, CH_4, and CO). These calculations used average temperatures to determine an integrated formula for fuel conversion.
- An alternative form of conversion was developed by looking at local Nusselt number (modified for the square channel configuration). This analysis is described on pages 15 and 16. The two methods show good agreement for C_7H_{14}conversion.
- Catalytic properties and functions are defined on pages 17-18, and the specific rate expression for oxidation of dilute CH_4 by supported palladium oxide (PdO) is described on page 19.
- Slow (in CPSTONE5.MCD and related to the rate of CH_4 oxidation) and moderate (in CPSTONE6.MCD and related to the rate of C_3H_6 oxidation) rate constants for C_7H_{14} oxidation are described on p. 19.
- The performance of the recuperator for conversion with temperature-dependent mass transfer properties and specific catalytic rates for C_7H_{14} and CH_4 are described on pages 20-21.

Performance of Upstream Monoliths

- The operating conditions for 200, 400, and 600 cells/in.^{2} honeycombs is described on pages 22-25.
- The pressure drop for three honeycombs (200, 400, and 600 cells/in.^{2}) is described on pages 22-23, and matched to the maximum specified conditions. From of these calculations, two honeycomb converter configurations, 400 cells/in.^{2} by 4 in. length and 600 cells/in.^{2} by 3.5 in. length, were chosen for mass transfer calculations.
- The effluent concentrations of added components are calculated for the constant temperature monoliths (400 cells/in.^{2} in CPSTONE5.MCD and 600 cells/in.^{2} in CPSTONE6.MCD) for the five operating conditions (cases) on pages 24-25, assuming very fast catalytic rates.
- Finally, on pages 25-27, the conversion of C_7H_{14} and CH_4 using finite catalytic rates are described for the honeycomb converters (400 cells/in.^{2} in CPSTONE5.MCD and 600 cells/in.^{2} in CPSTONE6.MCD).

RESULTS OF THE ANALYSIS

The principal results of the analysis of post turbine fuel component conversion are shown in the attached spreadsheet tables (CAPSTN5.XLS) and Mathcad documents (CPSTONE5.MCD and CPSTONE6.MCD). The main results of the analyses are summarized as follows:

Catalytic Recuperator

- The $\Delta P/P$ calculations seem to very closely fit your measured values. [redacted] We chose as the best calculation of pressure drop an 800 cells/in^2 x 7-in. with 10% additional added length to describe the chevron geometry of the recuperator foils.
- The estimated averaged wall temperatures, or skin temperatures, within the recuperator seemed a little low (< 50°F) based on [redacted] discussions of recuperator thermal efficiency. As a consequence, the cell size was increased to 600 cells/in^2 keeping the length the same (7 in. x 1.1) for a conservative calculation of mass transfer rates.
- For the mass transfer limited cases (assuming fast kinetics), virtually complete conversion CH_4 and CO is predicted (see Table of Results 1). Except at the highest power level, conversion of CH_4 and CO was essentially complete within the first inch or two of entry into the recuperator.
- For the transport-limited cases with C_7H_{14}, maximum conversions are low only for Case 5 (full power). Even in this case, 50 ppm would be converted to < 1 ppm (0.2 ppm) while concentrations entering the recuperator above 250 ppm would exit at levels above 1 ppm (500 ppm $\Rightarrow$ 2.1 ppm). The situation improves for the other cases (e.g., Case 4 gives 500 ppm $\Rightarrow$ 0.02 ppms while 5000 ppm $\Rightarrow$ 0.17 ppm).
- Conversions would be much higher for transport limited conversion in a the 800 cells/in.^{2} recuperator, as calculations with this cell size were found reproduce the observed pressure drop. In this case, the logarithm of the inlet concentration divided by the outlet concentration for all added components would be ~35 % greater with the smaller cell size.
- The step-wise calculation which includes the temperature on flow velocity and transport properties showed reasonably good agreement with the integrated calculation using average properties. This method gave lower overall conversion than the averaged property formulas, but the results were close. Perhaps the higher property values at the inlet, particularly the greater velocity, more than offset the lower transport values at the outlet side.
- CH_4 conversion is catalytically rate limited under all conditions (see Table of Results 1). Conversions were calculated to be very low, with a maximum conversion of ~66% under Case 1 and ~32% conversion under Case 5. These conversions would increase somewhat, perhaps by a factor of 2, with the use of a thicker coating (e.g., 25 μm vs. 10 μm).
- CO conversion is likely to exceed 99% in all operating conditions for the recuperator. This is because the kinetics of CO conversion are probably much faster than CH_4 and may well be close to the transport-limited case, at least through the (hotter) first several inches of the recuperator where most of the CO would be consumed.

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- The catalytic recuperator, C_7H_{14} rate determines its conversion in the recuperator conditions (see Table of Results 1). For the slower rates (derived from the rates for CH_4 oxidation) using the 600 cells/in.^{2} value for recuperator cell size, we find a range from 99.4% conversion under Case 1 to about 85.6% under Case 5. If twice the rate of combustion of propane is extrapolated to the higher temperatures of the recuperator, much higher C_7H_{14} conversions result, 99.98% under Case 1, and 96.4% under Case 5.

Catalytic Monoliths

- The pressure drop reaches maximum specifications for the 400 cells/in.^{2} honeycomb at 4-in. length. Maximum pressure drop would be reached in a shorter (~3.5 in. length) 600 cells/in.^{2} monolith. Both configurations were chosen for analysis (CPSTONE5.MCD for 400 cells/in.^{2} and CPSTONE6.MCD for 600 cells/in.^{2}).
- Transport-limited conversion shows excellent performance for methane and CO in all cases, including the full-power case, for both honeycomb configurations (see Table of Results 2).
- As for the recuperator, methane conversion is again reaction rate limited (see Table of Results 3), with conversions range from 93.8% under Case 1 with the 600 cells/in.^{2} monolith to only 31% conversion under Case 5 for the 400 cells/in.^{2} monolith.
- C_7H_{14} conversions under transport-limited conditions depends on the specific configuration (see Table of Results 2). For the 600 cells/in.^{2} monolith conversions are very high for Case 1, but fall to about 92% for Case 5. With the 400 cells/in.^{2} configuration, these fast kinetic transport-limited conversions fall to 87% conversion under Case 5.
- The reaction rate of C_7H_{14} strongly affects its conversion in either honeycomb monolith (see Table of Results 3). For the extrapolated propane kinetics at 600 cells/in.^{2}, 98% conversion is expected under Case 5, whereas the 400 cells/in.^{2} using the more conservative extrapolation using PdO methane kinetics, 86% conversion is expected under Case 5.

Effect of Washcoat Thermal Conductivity in a Recuperator

- The application of a thin washcoat of porous alumina gives a very slight *increase* in the overall heat transfer coefficient [redacted] CPSNALT2.MCD). The thermal conductivity of the washcoat, while significantly less than that of stainless 321, is greater than that of the gas phase boundary. Because the washcoat displaces the gas phase (creating a narrower channel) it causes a slight increase in overall heat transfer coefficient.

OVERALL CONCLUSIONS AND RECOMMENDATIONS

The conclusions and recommendations drawn from the results of the analysis is listed below:

1) The actual C_7H_{14} outlet concentration from the turbine are needed to assess the effluent emissions in the high-power case (Case 5) for either control strategy. Provided that fast catalytic rates can be provided in washcoats on either the recuperator or upstream monoliths, maximum conversions for C_7H_{14} under full power range from 99.6% (for an effective cell size of 600 cells/in^2) to > 99.9% (if the effective cell size is 800 cells/in^2).

2) The two methods (averaged properties and integrated formulas vs. local temperature dependent properties and finite difference integration) show good agreement for recuperator performance with infinitely fast catalytic reactions at the wall.

3) Clearly, it will be necessary to apply and measure specific catalytic rates for C_7H_{14} or gasoline to be sure that these estimated conversions could be achieved under actual operating conditions for either the catalytic recuperator or the upstream honeycomb monoliths.

4) Thin wash coats (< 20 μm) should have minimal effect on the transport of heat through the recuperator given the much greater resistance of the gas phase boundary layers.

5) For the current operating conditions, use of a standard 400 cells/in^2 x 4-in length catalytic monolith upstream of the recuperator is recommended.

6) If the recuperator temperature can be raised (~ 200°F) high conversions of CO, C_7H_{14}, and even CH_4 can be expected under all flow conditions. In this case it is possible that only the first 3 to 4 inches of the recuperator be wash coated with catalyst because the downstream wall temperatures are too cool to be effective.

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Inlet (added component) conc(ppm)	Recuperator - Transport only (assumes fast reaction kinetics) at 600 cells/in2														
	Case-1			Case-2			Case-3			Case-4			Case-5		
	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO	CH4	C7H14	CO
5000	2.011E-25	3.554E-05	5.555E-23	3.704E-19	0.002197	3.002E-17	1.373E-15	0.022964	5.542E-14	1.470E-12	0.1687	3.276E-11	2.818E-05	20.6392	1.467E-04
2000	8.046E-26	1.422E-05	2.222E-23	1.481E-19	8.787E-04	1.201E-17	5.492E-16	0.009186	2.217E-14	5.880E-13	0.0674683	1.310E-11	1.127E-05	8.2557	5.870E-05
1000	4.023E-26	7.108E-06	1.111E-23	7.407E-20	4.393E-04	6.003E-18	2.746E-16	0.004593	1.108E-14	2.940E-13	0.0337341	6.552E-12	5.637E-06	4.1278	2.935E-05
500	2.011E-26	3.554E-06	5.555E-24	3.704E-20	2.197E-04	3.002E-18	1.373E-16	0.002296	5.542E-15	1.470E-13	0.0168671	3.276E-12	2.818E-06	2.0639	1.467E-05
200	8.046E-27	1.422E-06	2.222E-24	1.481E-20	8.787E-05	1.201E-18	5.492E-17	9.186E-04	2.217E-15	5.880E-14	0.0067468	1.310E-12	1.127E-06	0.8256	5.870E-06
100	4.023E-27	7.108E-07	1.111E-24	7.407E-21	4.393E-05	6.003E-19	2.746E-17	4.593E-04	1.108E-15	2.940E-14	0.0033734	6.552E-13	5.637E-07	0.4128	2.935E-06
50	2.011E-27	3.554E-07	5.555E-25	3.704E-21	2.197E-05	3.002E-19	1.373E-17	2.296E-04	5.542E-16	1.470E-14	0.0016867	3.276E-13	2.818E-07	0.2064	1.467E-06
20	8.046E-28	1.422E-07	2.222E-25	1.481E-21	8.787E-06	1.201E-19	5.492E-18	9.186E-05	2.217E-16	5.880E-15	6.747E-04	1.310E-13	1.127E-07	0.082557	5.870E-07
10	4.023E-28	7.108E-08	1.111E-25	7.407E-22	4.393E-06	6.003E-20	2.746E-18	4.593E-05	1.108E-16	2.940E-15	3.373E-04	6.552E-14	5.637E-08	0.041278	2.935E-07
5	2.011E-28	3.554E-08	5.555E-26	3.704E-22	2.197E-06	3.002E-20	1.373E-18	2.296E-05	5.542E-17	1.470E-15	1.687E-04	3.276E-14	2.818E-08	0.020639	1.467E-07
2	8.046E-29	1.422E-08	2.222E-26	1.481E-22	8.787E-07	1.201E-20	5.492E-19	9.186E-06	2.217E-17	5.880E-16	6.747E-05	1.310E-14	1.127E-08	0.008256	5.870E-08
1	4.023E-29	7.108E-09	1.111E-26	7.407E-23	4.393E-07	6.003E-21	2.746E-19	4.593E-06	1.108E-17	2.940E-16	3.373E-05	6.552E-15	5.637E-09	0.004128	2.935E-08

Recuperator - C7H14 without reaction with T-dependence (step) and CH4and C7H14 with finite catalytic reaction rates at the wall (C7H14 rate = 10 x CH4 Rate - slow kinetics)

Inlet conc(ppm)	Case-1			Case-2			Case-3			Case-4			Case-5		
	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react	C7H14step	CH4react	C7H14react
5000	3.201E-04	1675.00	31.5850	0.012075	2065.00	82.9500	0.094050	2310.00	139.15	0.5350	2545.00	217.85	34.8400	3420.00	707.50
2000	1.280E-04	670.00	12.6340	0.004830	826.00	33.1800	0.037620	924.00	55.6600	0.2140	1018.00	87.1400	13.9360	1368.00	283.00
1000	6.402E-05	335.00	6.3170	0.002415	413.00	16.5900	0.018810	462.00	27.8300	0.1070	509.00	43.5700	6.9680	684.00	141.50
500	3.201E-05	167.50	3.1585	0.001208	206.50	8.2950	0.009405	231.00	13.9150	0.053500	254.50	21.7850	3.4840	342.00	70.7500
200	1.280E-05	67.0000	1.2634	0.000483	82.6000	3.3180	0.003762	92.4000	5.5660	0.021400	101.80	8.7140	1.3936	136.80	28.3000
100	6.402E-06	33.5000	0.6317	0.000242	41.3000	1.6590	0.001881	46.2000	2.7830	0.010700	50.9000	4.3570	0.6968	68.4000	14.1500
50	3.201E-06	16.7500	0.3159	0.000121	20.6500	0.8295	9.405E-04	23.1000	1.3915	0.005350	25.4500	2.1785	0.3484	34.2000	7.0750
20	1.280E-06	6.7000	0.1263	0.000048	8.2600	0.3318	3.762E-04	9.2400	0.5566	0.002140	10.1800	0.8714	0.1394	13.6800	2.8300
10	6.402E-07	3.3500	0.063170	2.415E-05	4.1300	0.1659	1.881E-04	4.6200	0.2783	0.001070	5.0900	0.4357	0.069680	6.8400	1.4150
5	3.201E-07	1.6750	0.031585	1.208E-05	2.0650	0.082950	9.405E-05	2.3100	0.1392	5.350E-04	2.5450	0.2179	0.034840	3.4200	0.7075
2	1.280E-07	0.6700	0.012634	4.830E-06	0.8260	0.033180	3.762E-05	0.9240	0.055660	2.140E-04	1.0180	0.0871	0.013936	1.3680	0.2830
1	6.402E-08	0.3350	0.006317	2.415E-06	0.4130	0.016590	1.881E-05	0.4620	0.027830	1.070E-04	0.5090	0.0436	0.006968	0.6840	0.1415

ln(yout/yin)

Case# :	1	2	3	4	5	
CH4:	-65.383	-50.957	-42.739	-35.763	-18.994	BL transport only with averaged intergated values
C7H14	-18.762	-14.638	-12.291	-10.297	-5.49	BL transport only with averaged intergated values
CO	-59.762	-46.562	-39.041	-32.659	-17.344	BL transport only with averaged intergated values
C7H14step	-16.56407	-12.933811	-10.88112	-9.142682	-4.966427	BL transport only with T-dependent properties and step-wise integration
CH4react	-1.0936247	-0.8843077	-0.77219	-0.675307	-0.379797	BL transport-restricted catalytic rates with T-dependent properties and step-wise integration
C7H14react	-5.0645109	-4.0989552	-3.581641	-3.133386	-1.955456	BL transport-restricted catalytic rates with T-dependent properties and step-wise integration

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Table of Results 2

Inlet (added component) conc(ppm)	Case-1 CH4	Case-1 C7H14	Case-1 CO	Case-2 CH4	Case-2 C7H14	Case-2 CO	Case-3 CH4	Case-3 C7H14	Case-3 CO	Case-4 CH4	Case-4 C7H14	Case-4 CO	Case-5 CH4	Case-5 C7H14	Case-5 CO
Transport only (assumes fast reaction kinetics) for a 600 cells/in2 x 3.5-in length square honeycomb monolith															
5000	7.960E-25	4.179E-04	2.470E-22	2.069E-18	0.017928	1.708E-16	9.839E-15	0.1545	3.802E-13	1.170E-11	0.9353	2.395E-10	2.773E-04	70.3859	0.001222
2000	3.184E-25	1.672E-04	9.878E-23	8.276E-19	0.007171	6.831E-17	3.936E-15	0.061810	1.521E-13	4.678E-12	0.3741	9.582E-11	1.109E-04	28.1544	4.890E-04
1000	1.592E-25	8.359E-05	4.939E-23	4.138E-19	0.003586	3.415E-17	1.968E-15	0.030905	7.604E-14	2.339E-12	0.1871	4.791E-11	5.546E-05	14.0772	2.445E-04
500	7.960E-26	4.179E-05	2.470E-23	2.069E-19	0.001793	1.708E-17	9.839E-16	0.015452	3.802E-14	1.170E-12	0.093528	2.395E-11	2.773E-05	7.0386	1.222E-04
200	3.184E-26	1.672E-05	9.878E-24	8.276E-20	0.000717	6.831E-18	3.936E-16	0.006181	1.521E-14	4.678E-13	0.037411	9.582E-12	1.109E-05	2.8154	4.890E-05
100	1.592E-26	8.359E-06	4.939E-24	4.138E-20	0.000359	3.415E-18	1.968E-16	0.003090	7.604E-15	2.339E-13	0.018706	4.791E-12	5.546E-06	1.4077	2.445E-05
50	7.960E-27	4.179E-06	2.470E-24	2.069E-20	0.000179	1.708E-18	9.839E-17	0.001545	3.802E-15	1.170E-13	0.009353	2.395E-12	2.773E-06	0.7039	1.222E-05
20	3.184E-27	1.672E-06	9.878E-25	8.276E-21	7.171E-05	6.831E-19	3.936E-17	6.181E-04	1.521E-15	4.678E-14	0.003741	9.582E-13	1.109E-06	0.2815	4.890E-06
10	1.592E-27	8.359E-07	4.939E-25	4.138E-21	3.586E-05	3.415E-19	1.968E-17	3.090E-04	7.604E-16	2.339E-14	0.001871	4.791E-13	5.546E-07	0.1408	2.445E-06
5	7.960E-28	4.179E-07	2.470E-25	2.069E-21	1.793E-05	1.708E-19	9.839E-18	1.545E-04	3.802E-16	1.170E-14	9.353E-04	2.395E-13	2.773E-07	0.070386	1.222E-06
2	3.184E-28	1.672E-07	9.878E-26	8.276E-22	7.171E-06	6.831E-20	3.936E-18	6.181E-05	1.521E-16	4.678E-15	3.741E-04	9.582E-14	1.109E-07	0.028154	4.890E-07
1	1.592E-28	8.359E-08	4.939E-26	4.138E-22	3.586E-06	3.415E-20	1.968E-18	3.090E-05	7.604E-17	2.339E-15	1.871E-04	4.791E-14	5.546E-08	0.014077	2.445E-07

Inlet conc(ppm)	Case-1 CH4	Case-1 C7H14	Case-1 CO	Case-2 CH4	Case-2 C7H14	Case-2 CO	Case-3 CH4	Case-3 C7H14	Case-3 CO	Case-4 CH4	Case-4 C7H14	Case-4 CO	Case-5 CH4	Case-5 C7H14	Case-5 CO
Transport only (assumes fast reaction kinetics) for a 400 cells/in2 x 4-in length square honeycomb monolith															
5000	3.307E-18	0.003426	2.617E-16	2.551E-13	0.090282	7.363E-12	1.616E-10	0.5882	2.615E-09	3.558E-08	2.81565014	3.550E-07	0.01476631	119.39	0.045698
2000	1.323E-18	0.001370	1.047E-16	1.021E-13	0.036113	2.945E-12	6.463E-11	0.2353	1.046E-09	1.423E-08	1.12626006	1.420E-07	0.00590653	47.7559	0.018279
1000	6.613E-19	6.852E-04	5.234E-17	5.103E-14	0.018058	1.473E-12	3.231E-11	0.1176	5.230E-10	7.115E-09	0.56313003	7.100E-08	0.00295326	23.8779	0.009140
500	3.307E-19	3.426E-04	2.617E-17	2.551E-14	0.009028	7.363E-13	1.616E-11	0.058825	2.615E-10	3.558E-09	0.28156501	3.550E-08	0.00147663	11.9390	0.004570
200	1.323E-19	1.370E-04	1.047E-17	1.021E-14	0.003612	2.945E-13	6.463E-12	0.023530	1.046E-10	1.423E-09	0.11262601	1.420E-08	5.907E-04	4.7756	0.001828
100	6.613E-20	6.852E-05	5.234E-18	5.103E-15	0.001806	1.473E-13	3.231E-12	0.011765	5.230E-11	7.115E-10	0.056313	7.100E-09	2.953E-04	2.3878	9.140E-04
50	3.307E-20	3.426E-05	2.617E-18	2.551E-15	9.029E-04	7.363E-14	1.616E-12	0.005882	2.615E-11	3.558E-10	0.0281565	3.550E-09	1.477E-04	1.1939	4.570E-04
20	1.323E-20	1.370E-05	1.047E-18	1.021E-15	3.612E-04	2.945E-14	6.463E-13	0.002353	1.046E-11	1.423E-10	0.0112626	1.420E-09	5.907E-05	0.4776	1.828E-04
10	6.613E-21	6.852E-06	5.234E-19	5.103E-16	1.806E-04	1.473E-14	3.231E-13	0.001176	5.230E-12	7.115E-11	0.0056313	7.100E-10	2.953E-05	0.2388	9.140E-05
5	3.307E-21	3.426E-06	2.617E-19	2.551E-16	9.029E-05	7.363E-15	1.616E-13	5.882E-04	2.615E-12	3.558E-11	0.00281565	3.550E-10	1.477E-05	0.1194	4.570E-05
2	1.323E-21	1.370E-06	1.047E-19	1.021E-16	3.612E-05	2.945E-15	6.463E-14	2.353E-04	1.046E-12	1.423E-11	0.00112626	1.420E-10	5.907E-06	0.047756	1.828E-05
1	6.613E-22	6.852E-07	5.234E-20	5.103E-17	1.806E-05	1.473E-15	3.231E-14	1.176E-04	5.230E-13	7.115E-12	5.631E-04	7.100E-11	2.953E-06	0.023878	9.140E-06

ln(yout/yin)

Case# :	1	2	3	4	5	
CH4-600	-64.0074	-49.2367	-40.7696	-33.689	-16.7076	BL transport only with averaged intergated values
C7H14-600	-16.2974	-12.5386	-10.3846	-8.5841	-4.2632	BL transport only with averaged intergated values
CO-600	-58.27	-44.8234	-37.1153	-30.6695	-15.2241	BL transport only with averaged intergated values
CH4-400	-48.7678	-37.5142	-31.0633	-25.6688	-12.7326	BL transport only with averaged intergated values
C7H14-400	-14.1935	-10.9219	-9.0478	-7.482	-3.7348	BL transport only with averaged intergated values
CO-400	-44.3966	-34.1518	-28.2792	-23.3684	-11.6029	BL transport only with averaged intergated values

CAPSTN5:XLS

T02280"E99EE660

Table of Results 3

[redacted]

Inlet (added		C7H14 with finite catalytic reaction rates at the wall (slow C7H14 rate = 10 x CH4 rate; moderate C7H14 rate = 2 x C3H8 rate)														
component)		Case-1			Case-2			Case-3			Case-4			Case-5	
conc(ppm)	Recup-m	600cpi-m	400cpi-s	Recup-m	600cpi-m	400cpi-s	Recup-m	600cpi-m	400cpi-s	Recup-m	600cpi-m	400cpi-s	Recup-m	600cpi-m	400cpi-s
5000	1.1680	0.001005	1.7905	5.7100	0.035610	11.1500	13.35	0.2715	31.6900	27.8200	14.9700	75.7500	180.18	99.6500	728.00
2000	0.4672	4.020E-04	0.7162	2.2840	0.014244	4.4600	5.3400	0.1086	12.6760	11.1280	5.9880	30.3000	72.0600	39.8600	291.20
1000	0.2336	2.010E-04	0.3581	1.1420	0.007122	2.2300	2.6700	0.054290	6.3380	5.5640	2.9940	15.1500	36.0300	19.9300	145.60
500	0.1168	1.005E-04	0.1791	0.5710	0.003561	1.1150	1.3350	0.027145	3.1690	2.7820	1.4970	7.5750	18.0150	9.9650	72.8000
200	0.046720	4.020E-05	0.071620	0.2284	0.001424	0.4460	0.5340	0.010858	1.2676	1.1128	0.5988	3.0300	7.2060	3.9860	29.1200
100	0.023360	2.010E-05	0.035810	0.1142	7.122E-04	0.2230	0.2670	0.005429	0.6338	0.5564	0.2994	1.5150	3.6030	1.9930	14.5600
50	0.011680	1.005E-05	0.017905	0.057100	3.561E-04	0.1115	0.1335	0.002715	0.3169	0.2782	0.1497	0.7575	1.8015	0.9965	7.2800
20	0.004672	4.020E-06	0.007162	0.022840	1.424E-04	0.044600	0.053400	0.001086	0.1268	0.1113	0.059880	0.3030	0.7206	0.3986	2.9120
10	0.002336	2.010E-06	0.003581	0.011420	7.122E-05	0.022300	0.026700	5.429E-04	0.063380	0.055640	0.029940	0.1515	0.3603	0.1993	1.4560
5	0.001168	1.005E-06	0.001791	0.005710	3.561E-05	0.011150	0.013350	2.715E-04	0.031690	0.027820	0.014970	0.075750	0.1802	0.099650	0.7280
2	4.672E-04	4.020E-07	7.162E-04	0.002284	1.424E-05	0.004460	0.005340	1.086E-04	0.012676	0.011128	0.005988	0.030300	0.072060	0.039860	0.2912
1	2.336E-04	2.010E-07	3.581E-04	0.001142	7.122E-06	0.002230	0.002670	5.429E-05	0.006338	0.005564	0.002994	0.015150	0.036030	0.019930	0.1456
		C7H14 without reaction and CH4 with finite catalytic reaction rates at the wall													
Inlet		Case-1			Case-2			Case-3			Case-4			Case-5	
conc(ppm)	C7H14	CH4H600	CH4H400	C7H14	CH4H600	CH4H400	C7H14	CH4H600	CH4H400	C7H14	CH4H600	CH4H400	C7H14	CH4H600	CH4H400
5000	3.201E-04	310.00	391.30	0.012075	590.00	705.50	0.094050	852.50	988.50	0.5350	1160.00	1310.50	34.8400	2846.50	2979.50
2000	1.280E-04	124.00	156.52	0.004830	236.00	282.20	0.037620	341.00	395.40	0.2140	464.00	524.20	13.9360	1138.60	1191.80
1000	6.402E-05	62.0000	78.2600	0.002415	118.00	141.10	0.018810	170.50	197.70	0.1070	232.00	262.10	6.9680	569.30	595.90
500	3.201E-05	31.0000	39.1300	0.001208	59.0000	70.5500	0.009405	85.2500	98.8500	0.053500	116.00	131.05	3.4840	284.65	297.95
200	1.280E-05	12.4000	15.6520	4.830E-04	23.6000	28.2200	0.003762	34.1000	39.5400	0.021400	46.4000	52.4200	1.3936	113.86	119.18
100	6.402E-06	6.2000	7.8260	2.415E-04	11.8000	14.1100	0.001881	17.0500	19.7700	0.010700	23.2000	26.2100	0.6968	56.9300	59.5900
50	3.201E-06	3.1000	3.9130	1.208E-04	5.9000	7.0550	9.405E-04	8.5250	9.8850	0.005350	11.6000	13.1050	0.3484	28.4650	29.7950
20	1.280E-06	1.2400	1.5652	4.830E-05	2.3600	2.8220	3.762E-04	3.4100	3.9540	0.002140	4.6400	5.2420	0.1394	11.3860	11.9180
10	6.402E-07	0.6200	0.7826	2.415E-05	1.1800	1.4110	1.881E-04	1.7050	1.9770	0.001070	2.3200	2.6210	0.069680	5.6930	5.9590
5	3.201E-07	0.3100	0.3913	1.208E-05	0.5900	0.7055	9.405E-05	0.8525	0.9885	5.350E-04	1.1600	1.3105	0.034840	2.8465	2.9795
2	1.280E-07	0.1240	0.1565	4.830E-06	0.2360	0.2822	3.762E-05	0.3410	0.3954	2.140E-04	0.4640	0.5242	0.013936	1.1386	1.1918
1	6.402E-08	0.062000	0.078260	2.415E-06	0.1180	0.1411	1.881E-05	0.1705	0.1977	1.070E-04	0.2320	0.2621	0.006968	0.5693	0.5959

				ln(yout/yin)			
Case# :	1	2	3	4	5		
C7H14Rs	2.34E-04	1.14E-03	2.67E-03	5.56E-03	3.60E-02		BL transport-restricted slower catalytic rates with T-dependent properties and step-wise integration
C7H14H600f	2.01E-07	7.12E-06	5.43E-05	2.99E-03	1.99E-02		BL transport-restricted moderate catalytic rates with T-dependent properties and step-wise integration
C7H14H400s	3.58E-04	2.23E-03	6.34E-03	1.52E-02	1.46E-01		BL transport-restricted slower catalytic rates with T-dependent properties and step-wise integration
C7H14R	-16.56407	-12.933811	-10.881122	-9.1426817	-4.966427		BL transport only with T-dependent properties and step-wise integration
CH4H600	0.062	0.118	0.1705	0.232	0.5693		BL transport-restricted catalytic rates with T-dependent properties and step-wise integration
CH4H400	0.07826	0.1411	0.1977	0.2621	0.5959		BL transport-restricted catalytic rates with T-dependent properties and step-wise integration

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Gas Properties and Constants

****

$cm \equiv 0.01 \cdot m$ $\qquad J \equiv kg \cdot m^2 \cdot sec^{-2}$ $\qquad W \equiv J \cdot sec^{-1}$ $\qquad Pref \equiv 1 \cdot atm$

$N \equiv kg \cdot m \cdot sec^{-2}$ $\qquad Pa \equiv N \cdot m^{-2}$ $\qquad atm \equiv 101300 \cdot Pa$ $\qquad \mu m \equiv 0.000001 \cdot m$

$R \equiv 8.3143 \cdot \frac{J}{K}$ $\qquad Rc \equiv 8.3143 \cdot J \cdot mole^{-1} \cdot K^{-1}$

****

n	Gas	MolWt	σ(LJ)	ε(LJ)
0	CH4	$MW_0 := 16.044 \cdot gm$	$\sigma_0 := 3.785 \cdot 10^{-10} \cdot m$	$\varepsilon_0 := 148.6 \cdot K$
1	O2	$MW_1 := 31.999 \cdot gm$	$\sigma_1 := 3.464 \cdot 10^{-10} \cdot m$	$\varepsilon_1 := 106.7 \cdot K$
2	N2	$MW_2 := 28.018 \cdot gm$	$\sigma_2 := 3.798 \cdot 10^{-10} \cdot m$	$\varepsilon_2 := 71.4 \cdot K$
3	CO2	$MW_3 := 44.010 \cdot gm$	$\sigma_3 := 3.941 \cdot 10^{-10} \cdot m$	$\varepsilon_3 := 195.2 \cdot K$
4	H2O	$MW_4 := 18.015 \cdot gm$	$\sigma_4 := 2.641 \cdot 10^{-10} \cdot m$	$\varepsilon_4 := 809.1 \cdot K$

5 C7H14 methyl-cyclohexane $\qquad Tc7 := 572.2 \cdot K$ $\qquad Tb7 := 374.1 \cdot K$ $\qquad Pc7 := 3.47 \cdot 10^6 \cdot Pa$ $\qquad Vc7 := 368$

$$\varepsilon_5 := \frac{Tc7}{1.2593} \qquad \sigma_5 := Vc7^{\frac{1}{3}} \cdot 10^{-10} \cdot m$$

$MW_5 := 98.189 \cdot gm$ $\qquad \sigma_5 = 7.1661 \cdot 10^{-10} \cdot m$ $\qquad \varepsilon_5 = 454.3794 \cdot K$

6 CO $\qquad MW_6 := 28.01 \cdot gm$ $\qquad \sigma_6 := 3.69 \cdot 10^{-10} \cdot m$ $\qquad \varepsilon_6 := 91.7 \cdot K$

****

Define constants for transport integrals:

$\sigma\mu a_0 := 1.16145$ $\qquad \sigma\mu b_0 := 0.14874$ $\qquad \sigma Da_0 := 1.06036$ $\qquad \sigma Db_0 := 0.1561$

$\sigma\mu a_1 := 0.52487$ $\qquad \sigma\mu b_1 := 0.7732$ $\qquad \sigma Da_1 := 0.193$ $\qquad \sigma Db_1 := 0.47635$

$\sigma\mu a_2 := 2.16178$ $\qquad \sigma\mu b_2 := 2.43787$ $\qquad \sigma Da_2 := 1.03587$ $\qquad \sigma Db_2 := 1.52996$

$\sigma Da_3 := 1.76474$ $\qquad \sigma Db_3 := 3.89411$

Define transport integrals:

$$\Omega\mu(T) := \sigma\mu a_0 \cdot \exp(-\sigma\mu b_0 \cdot \ln(T)) + \sum_{i\mu=1}^{2} \sigma\mu a_{i\mu} \cdot \exp(-\sigma\mu b_{i\mu} \cdot T) \qquad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) := \sigma Da_0 \cdot \exp(-\sigma Db_0 \cdot \ln(T)) + \sum_{i\mu=1}^{3} \sigma Da_{i\mu} \cdot \exp(-\sigma Db_{i\mu} \cdot T) \qquad \Omega D(3) = 0.95002$$

****

Set Inlet Conditions:

$P := 1\cdot atm$

$\phi := 0.1$

$yadc7 := 0.0021859$

This value for yadc7 was determined via enthalpy functions [redacted] for temperature rise from 1000F to 1511F.

$yeqc7 := \phi\cdot\frac{0.205}{14}$

$\phi eq := \phi\cdot\frac{yadc7}{yeqc7}$

The value for yeq was determine for a given equilvalence ratio of 0.1 in moist air

$yeqc7 = 0.001464$

$\phi eq = 0.149281$

Define gas composition with C7H14 fuel using moist (2%) air:

$$y7(y0,x) := \frac{\begin{bmatrix} 0 \\ (1-y0)\cdot 0.205 - 10.5\cdot y0\cdot x \\ (1-y0)\cdot 0.775 \\ 7\cdot(y0\cdot x) \\ (1-y0)\cdot 0.02 + 7\cdot y0\cdot x \\ y0\cdot(1-x) \\ 0 \end{bmatrix}}{1+2.5\cdot y0\cdot x}$$

$yeq := y7(yeqc7,1)$

$$yeq = \begin{bmatrix} 0 \\ 0.188634 \\ 0.771043 \\ 0.010213 \\ 0.03011 \\ 0 \\ 0 \end{bmatrix}$$

$yad := y7(yadc7,1)$

$$yad = \begin{bmatrix} 0 \\ 0.180613 \\ 0.769103 \\ 0.015218 \\ 0.035066 \\ 0 \\ 0 \end{bmatrix}$$

Define functions for evaluation of mixture properties (ideal gas) for complete fuel conversion and a given temperature.

Density and average molecular weight:

$$\rho mix(T) := \left(\sum_{kk=0}^{6} yeq_{kk}\cdot MW_{kk}\right)\cdot\frac{P}{R\cdot T}$$

$$MWmix := \left(\sum_{kk=0}^{6} yeq_{kk}\cdot MW_{kk}\right)$$

$\rho mix(300\cdot K) = 1.162787\cdot kg\cdot m^{-3}$

$MWmix = 28.631\cdot gm$

****

Define diffusion coefficients for specific binary diffusion pairs:

$$\mathrm{Diff}(n,m,T) := 1.8829\cdot 10^{-27}\cdot\frac{\left[\left(\frac{1}{MW_n}+\frac{1}{MW_m}\right)\cdot T^3\right]^{0.5}}{\left(\frac{\sigma_n+\sigma_m}{2}\right)^2\cdot\Omega D\left[\frac{T}{\left(\varepsilon_n\cdot\varepsilon_m\right)^{0.5}}\right]\cdot\frac{P}{Pref}}\cdot 10^8\cdot gm^{0.5}\cdot cm^4\cdot sec^{-1}\cdot K^{-1.5}$$

$\mathrm{Diff}(0,2,300\cdot K) = 0.2225\cdot sec^{-1}\cdot cm^2$ $\quad$ $\mathrm{Diff}(2,6,300\cdot K) = 0.207\cdot sec^{-1}\cdot cm^2$

Define functions for use with various fuel-air mixtures:

$$\mathrm{Dch4}(T) := \frac{1}{\displaystyle\sum_{jgas=1}^{4}\frac{yeq_{jgas}}{\mathrm{Diff}(0,jgas,T)}}$$

$\mathrm{Dch4}(298\cdot K) = 2.1912\cdot 10^{-5}\cdot m^2\cdot sec^{-1}$

$$\mathrm{Dc7h14}(T) := \frac{1}{\displaystyle\sum_{jgas=1}^{4}\frac{yeq_{jgas}}{\mathrm{Diff}(5,jgas,T)}}$$

$\mathrm{Dc7h14}(298\cdot K) = 5.8372\cdot 10^{-6}\cdot m^2\cdot sec^{-1}$

$$\mathrm{Dco}(T) := \frac{1}{\displaystyle\sum_{jgas=1}^{4}\frac{yeq_{jgas}}{\mathrm{Diff}(6,jgas,T)}}$$

$\mathrm{Dco}(298\cdot K) = 2.0451\cdot 10^{-5}\cdot m^2\cdot sec^{-1}$

****

Display gas mixture properties

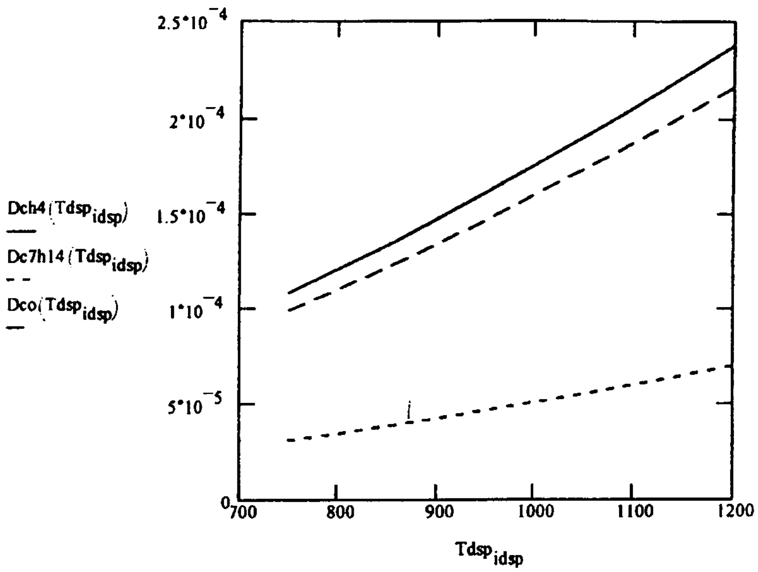
$idsp := 0..9$

$Tin := \left[(1000-32)\cdot\frac{5}{9}+273.15\right]\cdot K$ $\quad$ $Tin = 810.9278\cdot K$

$Tdsp_{idsp} := (750+50\cdot idsp)\cdot K$

$Tout := \left[(1511-32)\cdot\frac{5}{9}+273.15\right]\cdot K$ $\quad$ $Tout = 1094.8167\cdot K$

****



$Tdsp_{idsp}$	$Dch4(Tdsp_{idsp})$	$Dc7h14(Tdsp_{idsp})$	$Dco(Tdsp_{idsp})$
$7.5\cdot10^{2}\cdot K$	$1.082\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$3.1097\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$9.8836\cdot10^{-5}\cdot m^2\cdot sec^{-1}$
$8\cdot10^{2}\cdot K$	$1.2064\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$3.4776\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.101\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$8.5\cdot10^{2}\cdot K$	$1.3359\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$3.8613\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.2184\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$9\cdot10^{2}\cdot K$	$1.4705\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$4.2603\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.3402\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$9.5\cdot10^{2}\cdot K$	$1.61\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$4.6743\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.4665\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$1\cdot10^{3}\cdot K$	$1.7543\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$5.1031\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.5972\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$1.05\cdot10^{3}\cdot K$	$1.9033\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$5.5462\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.7322\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$1.1\cdot10^{3}\cdot K$	$2.057\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$6.0035\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$1.8714\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$1.15\cdot10^{3}\cdot K$	$2.2152\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$6.4746\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$2.0148\cdot10^{-4}\cdot m^2\cdot sec^{-1}$
$1.2\cdot10^{3}\cdot K$	$2.378\cdot10^{-4}\cdot m^2\cdot sec^{-1}$	$6.9593\cdot10^{-5}\cdot m^2\cdot sec^{-1}$	$2.1624\cdot10^{-4}\cdot m^2\cdot sec^{-1}$

Define interpolation formulas for Dch4, Dc7h14, and Dco vs. T(K) via Jandel Scientific's Tablecurve program

$$Dch4T(T) := \exp\left(-10.623294 + 1.6259688\cdot\ln\left(\frac{T}{K}\right) - \frac{46.41736\cdot K}{T}\right)\cdot\frac{cm^2}{sec}$$

$Dch4(1000\cdot K) = 1.75426\cdot sec^{-1}\cdot cm^2$

$Dch4T(1000\cdot K) = 1.75432\cdot sec^{-1}\cdot cm^2$

$$Dc7h14T(T) := \exp\left(-11.822189 + 1.6260138\cdot\ln\left(\frac{T}{K}\right) - \frac{82.65375\cdot K}{T}\right)\cdot\frac{cm^2}{sec}$$

$Dc7h14(1000\cdot K) = 0.51031\cdot sec^{-1}\cdot cm^2$

$Dc7h14T(1000\cdot K) = 0.51031\cdot sec^{-1}\cdot cm^2$

$$DcoT(T) := \exp\left(-10.831955 + 1.6394196\cdot\ln\left(\frac{T}{K}\right) - 24.53899\cdot\frac{K}{T}\right)\cdot cm^2\cdot sec^{-1}$$

$Dco(1000\cdot K) = 1.59722\cdot sec^{-1}\cdot cm^2$

$DcoT(1000\cdot K) = 1.59714\cdot sec^{-1}\cdot cm^2$

****

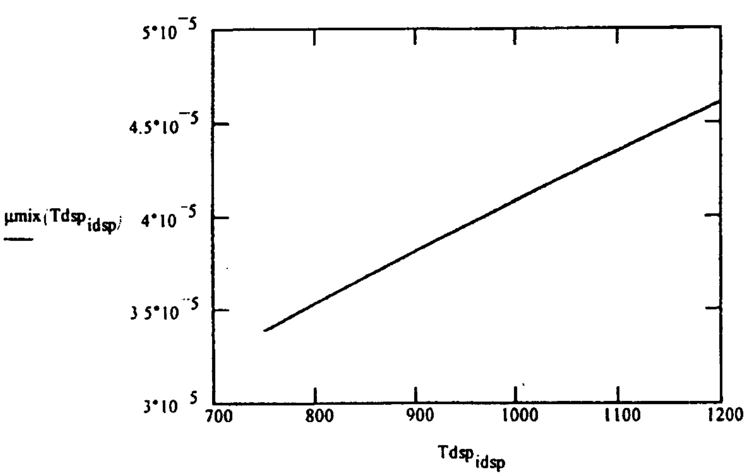
Define viscosity functions for major constituents:

$$\mu(T) := \begin{bmatrix} 2.6693\cdot 10^{-26}\cdot\dfrac{(MW_0\cdot T)^{0.5}}{(\sigma_0)^2\cdot\Omega\mu\left(\dfrac{T}{\varepsilon_0}\right)}\cdot\dfrac{10^5\cdot cm}{sec}\cdot\left(\dfrac{gm}{K}\right)^{0.5} \\ \dfrac{(MW_1\cdot T)^{0.5}}{(\sigma_1)^2\cdot\Omega\mu\left(\dfrac{T}{\varepsilon_1}\right)}\cdot\left[2.6693\cdot 10^{-26}\cdot\left(\dfrac{10^5\cdot cm}{sec}\right)\cdot\left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{(MW_2\cdot T)^{0.5}}{(\sigma_2)^2\cdot\Omega\mu\left(\dfrac{T}{\varepsilon_2}\right)}\cdot\left[2.6693\cdot 10^{-26}\cdot\left(\dfrac{10^5\cdot cm}{sec}\right)\cdot\left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{(MW_3\cdot T)^{0.5}}{(\sigma_3)^2\cdot\Omega\mu\left(\dfrac{T}{\varepsilon_3}\right)}\cdot\left[2.6693\cdot 10^{-26}\cdot\left(\dfrac{10^5\cdot cm}{sec}\right)\cdot\left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{1.116\cdot(MW_4\cdot T)^{0.5}}{(3.115\cdot 10^{-8}\cdot cm)^2\cdot\Omega\mu\left(\dfrac{T}{514\cdot K}\right)}\cdot\left[2.6693\cdot 10^{-26}\cdot\left(\dfrac{10^5\cdot cm}{sec}\right)\cdot\left(\dfrac{gm}{K}\right)^{0.5}\right] \end{bmatrix}$$

$$\mu(300\cdot K) = \begin{bmatrix} 1.10281\cdot 10^{-5} \\ 2.0603\cdot 10^{-5} \\ 1.76981\cdot 10^{-5} \\ 1.51851\cdot 10^{-5} \\ 1.06784\cdot 10^{-5} \end{bmatrix}\cdot kg\cdot m^{-1}\cdot sec^{-1}$$

$$\mu mix(T) := \sum_{n=1}^{4}\frac{yeq_n\cdot\mu(T)_n}{\displaystyle\sum_{m=1}^{4} yeq_m\cdot\left[\frac{\left[1+\left(\dfrac{\mu(T)_n}{\mu(T)_m}\right)^{0.5}\cdot\left(\dfrac{MW_m}{MW_n}\right)^{0.25}\right]^2}{\left[8\cdot\left(1+\dfrac{MW_n}{MW_m}\right)\right]^{0.5}}\right]}$$

$$yeq = \begin{bmatrix} 0 \\ 0.1886 \\ 0.771 \\ 0.0102 \\ 0.0301 \\ 0 \\ 0 \end{bmatrix}$$



$Tdsp_{idsp}$	$\mu mix(Tdsp_{idsp})$
750·K	$3.3875\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
800·K	$3.5348\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
850·K	$3.6787\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
900·K	$3.8194\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
950·K	$3.9573\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
1000·K	$4.0926\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
1050·K	$4.2254\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
1100·K	$4.356\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
1150·K	$4.4844\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$
1200·K	$4.6108\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$

$$\mu mixT(T) := \exp\left(-0.6984944 + 0.640549 \cdot \ln\left(\frac{T}{K}\right) + \frac{-14.50559 \cdot K}{T}\right) \cdot 10^{-6} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$\mu mix(1000 \cdot K) = 4.0926 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$ $\qquad$ $\mu mixT(1000 \cdot K) = 4.09256 \cdot 10^{-5} \cdot kg \cdot m^{-1} \cdot sec^{-1}$

****

Define thermal conductivity functions for light molecules

$igas := 0, 1 .. 4$

$$a\lambda := \begin{bmatrix} -1.869 \\ -.3273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda := \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda := \begin{bmatrix} 1.179 \cdot 10^{-4} \\ -(3.743 \cdot 10^{-5}) \\ -(5.067 \cdot 10^{-5}) \\ 5.477 \cdot 10^{-6} \\ 1.801 \cdot 10^{-4} \end{bmatrix} \quad d\lambda := \begin{bmatrix} -(3.614 \cdot 10^{-8}) \\ 9.732 \cdot 10^{-9} \\ 1.504 \cdot 10^{-8} \\ -(1.053 \cdot 10^{-8}) \\ -(9.1 \cdot 10^{-8}) \end{bmatrix} \begin{matrix} CH4 \\ O2 \\ N2 \\ CO2 \\ H2O \end{matrix}$$

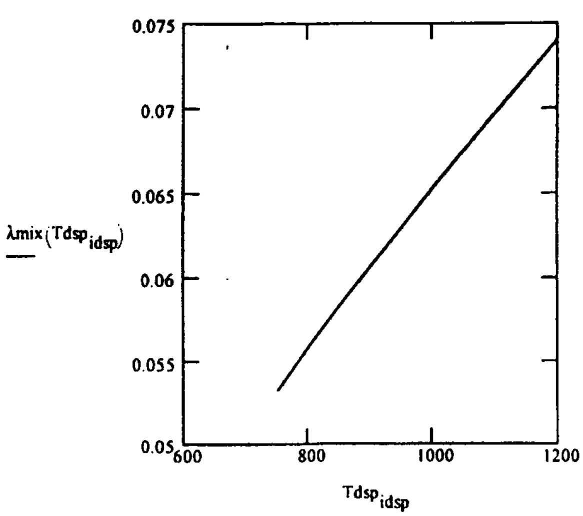
$$\lambda(i,T) := \left[a\lambda_i + b\lambda_i \cdot \frac{T}{K} + c\lambda_i \cdot \left(\frac{T}{K}\right)^2 + d\lambda_i \cdot \left(\frac{T}{K}\right)^3\right] \cdot 0.00001 \cdot \frac{W}{cm \cdot K}$$

$\lambda(igas, 1000 \cdot K)$
$0.16716 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.07163 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.06292 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.06788 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$0.08631 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$

W/m/K

$$\lambda mix(T) := \sum_{i=1}^{4} \frac{yeq_i \cdot \lambda(i,T)}{\sum_{j=1}^{4} yeq_j \cdot \left[\frac{\left[1 + \left(\frac{\mu(T)_i}{\mu(T)_j}\right)^{0.5} \cdot \left(\frac{MW_j}{MW_i}\right)^{0.25}\right]^2}{\left[8 \cdot \left(1 + \frac{MW_i}{MW_j}\right)\right]^{0.5}}\right]}$$

$$\lambda mix(1000 \cdot K) = 0.000653 \cdot \frac{W}{cm \cdot K}$$



$Tdsp_{idsp}$	$\lambda mix(Tdsp_{idsp})$
$7.5 \cdot 10^2 \cdot K$	$0.05323 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$8 \cdot 10^2 \cdot K$	$0.055775 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$8.5 \cdot 10^2 \cdot K$	$0.058242 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$9 \cdot 10^2 \cdot K$	$0.060641 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$9.5 \cdot 10^2 \cdot K$	$0.06298 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1 \cdot 10^3 \cdot K$	$0.065268 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.05 \cdot 10^3 \cdot K$	$0.067512 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.1 \cdot 10^3 \cdot K$	$0.069721 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.15 \cdot 10^3 \cdot K$	$0.071904 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$
$1.2 \cdot 10^3 \cdot K$	$0.074069 \cdot kg \cdot m \cdot sec^{-3} \cdot K^{-1}$

$$\lambda mixT(T) := \exp\left(-7.073383 + 0.6397005 \cdot \ln\left(\frac{T}{K}\right) + \frac{-65.2387 \cdot K}{T}\right) \cdot W \cdot m^{-1} \cdot K^{-1}$$

$\lambda mix(1000 \cdot K) = 0.0653 \cdot m^{-1} \cdot K^{-1} \cdot W$ $\qquad$ $\lambda mixT(1000 \cdot K) = 0.0659 \cdot m^{-1} \cdot K^{-1} \cdot W$

****

Define heat capacities:

$$Cpcoef := \begin{bmatrix} 19.25 & .05213 & 0.00001197 & -0.00000001132 \\ 28.11 & -0.000368 & 0.00001746 & -0.00000001065 \\ 31.15 & -0.01357 & 0.0000268 & -0.00000001168 \\ 19.8 & 0.07344 & -0.00005602 & 0.00000001715 \\ 32.24 & 0.001924 & 0.00001055 & -0.000000003596 \\ -76.19 & 0.7867 & -0.0004204 & 0.00000007516 \end{bmatrix}$$

$$Cp(igas, T) := \sum_{jj=0}^{3} Cpcoef_{igas,jj} \cdot \left(\frac{T}{K}\right)^{jj} \cdot \frac{J}{K}$$

J/mol/K

$jj := 0..3$

$Cp(0, 300 \cdot K) = 35.6607 \cdot K^{-1} \cdot J$ $\qquad$ $Cp(5, 300 \cdot K) = 124.0133 \cdot K^{-1} \cdot J$

$$Cpmix(T) := \sum_{jk=1}^{4} Cp(jk, T) \cdot yeq_{jk}$$

$Cpmix(998 \cdot K) = 33.5144 \cdot J \cdot K^{-1}$

$$Cpcfmix_{jj} := \sum_{jk=1}^{4} Cpcoef_{jk,jj} \cdot yeq_{jk} \cdot \frac{J}{K}$$

$$Cpcfmix = \begin{bmatrix} 30.493459 \\ -0.009725 \\ 2.370305 \cdot 10^{-5} \\ -1.094786 \cdot 10^{-8} \end{bmatrix} \cdot kg \cdot m^2 \cdot sec^{-2} \cdot 1$$

$$CpmixT(T) := \sum_{jj=0}^{3} Cpcfmix_{jj} \cdot \left(\frac{T}{K}\right)^{jj}$$

$Cpmix(1000 \cdot K) = 33.52413 \cdot kg \cdot m^2 \cdot sec^{-2} \cdot K^{-1}$

$CpmixT(1000 \cdot K) = 33.52413 \cdot kg \cdot m^2 \cdot sec^{-2} \cdot K^{-1}$

$igas := 0, 1..6$ $\qquad$ $P = 1.013 \cdot 10^5 \cdot Pa$

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Define momentum and thermal diffusivities:

$\alpha(\text{igas},T) := \dfrac{\lambda(\text{igas},T)\cdot R\cdot T}{Cp(\text{igas},T)\cdot P}$ $\qquad \alpha(0,300\cdot K) = 0.2344\cdot sec^{-1}\cdot cm^2$

$\alpha mix(T) := \dfrac{\lambda mixT(T)\cdot R\cdot T}{CpmixT(T)\cdot P}$ $\qquad \alpha mix(1000\cdot K) = 1.6132\cdot sec^{-1}\cdot cm^2$

$\upsilon mix(T) := \dfrac{\mu mixT(T)}{\rho mix(T)}$ $\qquad \upsilon mix(1000\cdot K) = 1.1732\cdot sec^{-1}\cdot cm^2$

$\upsilon mixT(T) := \dfrac{\mu mixT(T)}{\rho mix(T)}$ $\qquad \rho mix(1000\cdot K) = 3.48836\cdot 10^{-4}\cdot gm\cdot cm^{-3}$

$\rho mixT(T) := \rho mix(T)$

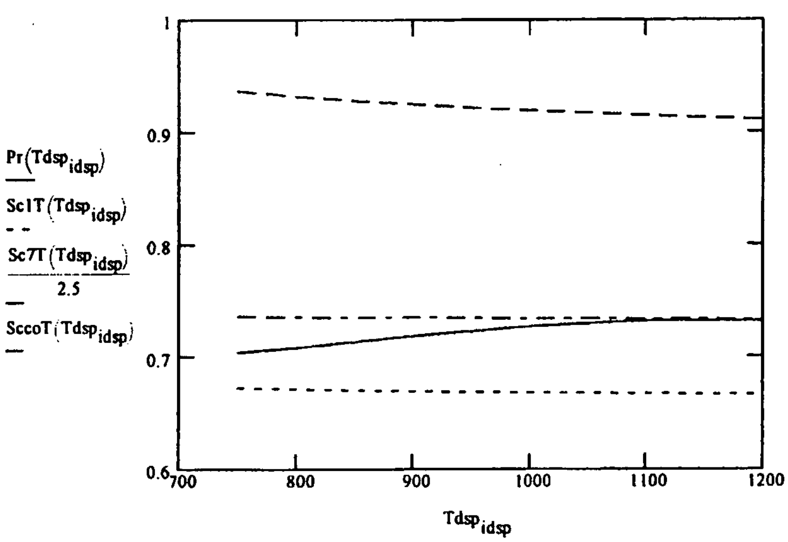
$Dch4T(1000\cdot K) = 1.7543\cdot sec^{-1}\cdot cm^2$ $\qquad Dc7h14T(1000\cdot K) = 0.5103\cdot sec^{-1}\cdot cm^2$

Define Prandl, Schmidt, and Lewis numbers

$Pr(T) := \dfrac{\upsilon mix(T)}{\alpha mix(T)}$ $\qquad Pr(1000\cdot K) = 0.7272$

$Sc1T(T) := \dfrac{\upsilon mix(T)}{Dch4T(T)}$ $\qquad Sc1T(1000\cdot K) = 0.6688$ $\qquad Sc7T(T) := \dfrac{\upsilon mix(T)}{Dc7h14T(T)}$ $\qquad Sc7T(1000\cdot K) = 2.299$

$SccoT(T) := \dfrac{\upsilon mix(T)}{DcoT(T)}$ $\qquad SccoT(1000\cdot K) = 0.7346$



These relations have weak temperature dependence and (presumably) very weak dependence on composition

This ends the extended section that defines gas properties for the combustion mixtures.

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Honeycombs: Represent as square channel metal alloy wall 0.003 mil, uncoated; 0.004 mil coated

$dwalluc := 0.003 \cdot in$ $\quad dwalluc = 7.62 \cdot 10^{-5} \cdot m$ $\quad dwallc := 0.004 \cdot in$ $\quad dwallc = 1.016 \cdot 10^{-4} \cdot m$

$Cells1 := 100 \cdot in^{-2}$ $\quad dwall1 := dwallc$ $\quad Cells2 := 200 \cdot in^{-2}$ $\quad dwall2 := dwallc$

$dcell1 := (Cells1)^{-0.5} - dwall1$ $\quad dcell2 := (Cells2)^{-0.5} - dwall2$

$dcell1 = 0.2438 \cdot cm$ $\quad ks1 := 0.002 \cdot cm$ $\quad dcell2 = 0.1694 \cdot cm$ $\quad ks2 := 0.002 \cdot cm$

$\varepsilon cell1 := dcell1^2 \cdot Cells1$ $\quad \varepsilon cell1 = 0.9216$ $\quad \varepsilon cell2 := dcell2^2 \cdot Cells2$ $\quad \varepsilon cell2 = 0.89006$

$Cells4 := 400 \cdot in^{-2}$ $\quad dwall4 := dwallc$ $\quad Cells6 := 600 \cdot in^{-2}$ $\quad dwall6 := dwalluc$

$dcell4 := (Cells4)^{-0.5} - dwall4$ $\quad dcell4 = 0.1168 \cdot cm$ $\quad dcell6 := (Cells6)^{-0.5} - dwall6$ $\quad dcell6 = 0.0961 \cdot cm$

$dcell4 = 0.1168 \cdot cm$ $\quad ks4 := 0.001 \cdot cm$ $\quad dcell6 = 0.0961 \cdot cm$ $\quad ks6 := 0 \cdot cm$

$\varepsilon cell4 := dcell4^2 \cdot Cells4$ $\quad \varepsilon cell4 = 0.8464$ $\quad \varepsilon cell6 := dcell6^2 \cdot Cells6$ $\quad \varepsilon cell6 = 0.85843$

$Cells8 := 800 \cdot in^{-2}$ $\quad dwall8 := dwalluc$

$dcell8 := (Cells8)^{-0.5} - dwall8$ $\quad dcell8 = 0.0822 \cdot cm$

$dcell8 = 0.0822 \cdot cm$ $\quad ks8 := 0 \cdot cm$

$\varepsilon cell8 := dcell8^2 \cdot Cells8$ $\quad \varepsilon cell8 = 0.83749$

****

Define recuperator and monolith configurations:

$dreco := 17 \cdot in$ $\quad dreco = 43.18 \cdot cm$ $\quad Lrec := 7 \cdot in$

$dreci := 6 \cdot in$ $\quad dreci = 15.24 \cdot cm$ $\quad Lrec = 17.78 \cdot cm$

$\delta d := 1.375 \cdot in$ **Add space for mounting and insulation?**

$dhco := dreco - \delta d$ $\quad dhco = 39.6875 \cdot cm$ $\quad Lhc := 4 \cdot in$

$dhci := dreci + \delta d$ $\quad dhci = 18.7325 \cdot cm$ $\quad Lhc = 10.16 \cdot cm$

$$Shc := \pi \cdot \frac{dhco^2 - dhci^2}{4} \qquad Shc = 0.0961 \cdot m^2$$

$$Srecup := 0.0958 \cdot m^2 \qquad \frac{Srecup}{Shc} = 0.9964$$

****

Define initial combustion conditions

$jcase := 0, 1 .. 4$

$$case := \begin{pmatrix} 0.2 & 1350 & 340 \\ 0.26 & 1350 & 390 \\ 0.314 & 1350 & 440 \\ 0.38 & 1350 & 490 \\ 0.72 & 1190 & 675 \end{pmatrix}$$

Mass flow (lb/sec)
Recup T inlet (F)
Recup T outlet (F)

$$TKF(T) := \left(\frac{T}{K} - 273.15\right) \cdot \frac{9}{5} + 32$$

$$TFK(t) := \frac{(t - 32) \cdot 5 \cdot K}{9} + 273.15 \cdot K$$

$Prec := 1\cdot atm$ $\qquad$ $Phc := 1\cdot atm$

$mf_{jcase+1} := case_{jcase,0}\cdot 0.454\cdot kg\cdot sec^{-1}$ $\qquad$ $Trecin_{jcase+1} := TFK\left(case_{jcase,1}\right)$ $\qquad$ $Trecout_{jcase+1} := TFK\left(case_{jcase,2}\right)$

$$mf = \begin{bmatrix} 0 \\ 0.0908 \\ 0.118 \\ 0.1426 \\ 0.1725 \\ 0.3269 \end{bmatrix}\cdot kg\cdot sec^{-1} \qquad Trecin = \begin{bmatrix} 0 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 1005.37 \\ 916.48 \end{bmatrix}\cdot K \qquad Trecout = \begin{bmatrix} 0 \\ 444.26 \\ 472.04 \\ 499.82 \\ 527.59 \\ 630.37 \end{bmatrix}\cdot K$$

$$Urec_{jcase+1} := \frac{mf_{jcase+1}}{\rho mix\left(Trecin_{jcase+1}\right)\cdot \frac{Srecup}{2}} \qquad Urec = \begin{bmatrix} 0 \\ 5.4633 \\ 7.1023 \\ 8.5774 \\ 10.3803 \\ 17.929 \end{bmatrix}\cdot m\cdot sec^{-1} \qquad Grec_{jcase+1} := \frac{mf_{jcase+1}}{\left(\frac{Srecup}{2}\right)}$$

Only half of the recuperator cross section is available for exhuast gas flow

$$Uhc2_{jcase+1} := \frac{mf_{jcase+1}}{\rho mix\left(Trecin_{jcase+1}\right)\cdot Shc\cdot \varepsilon cell2} \qquad Uhc4_{jcase+1} := Uhc2_{jcase+1}\cdot \frac{\varepsilon cell2}{\varepsilon cell4} \qquad Uhc6_{jcase+1} := Uhc2_{jcase+1}\cdot \frac{\varepsilon cell2}{\varepsilon cell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix}\cdot m\cdot sec^{-1} \qquad Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix}\cdot m\cdot sec^{-1}$$

$$Tavg := \frac{Trecin + Trecout}{2} \qquad Tavg = \begin{bmatrix} 0 \\ 724.8167 \\ 738.7056 \\ 752.5944 \\ 766.4833 \\ 773.4278 \end{bmatrix}\cdot K$$

Define average temperature etc/ for estimated ΔP and ΔT in the recuperator

$$\rho mixrec(T) := \frac{MWmix\cdot Prec}{R\cdot T} \qquad \rho mixrec\left(Tavg_1\right) = 0.4813\cdot kg\cdot m^{-3}$$

****

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$\mathrm{Rerec6}(G,T) := \frac{G\cdot \mathrm{dcell6}}{\mu\mathrm{mixT}(T)} \qquad \mathrm{Rerec6}\left(\mathrm{Grec}_1,\mathrm{Tavg}_1\right) = 54.9906$$

$$\mathrm{Rerec8}(G,T) := \frac{G\cdot \mathrm{dcell8}}{\mu\mathrm{mixT}(T)} \qquad \mathrm{Rerec8}\left(\mathrm{Grec}_1,\mathrm{Tavg}_1\right) = 47.0389$$

For laminar flow with entrance effect (adapted from Kays & Crawford, "Convective Heat and Mass Transfer"):

$$\mathrm{cfricrec8}(G,T,z) := \frac{14.227}{\mathrm{Rerec8}(G,T)}\cdot\left[1 + 0.046263\cdot\left(\mathrm{Rerec8}(G,T)\cdot\frac{\mathrm{dcell8}}{z}\right)\right]^{0.45363}$$

$$\mathrm{cfricrec6}(G,T,z) := \frac{14.227}{\mathrm{Rerec6}(G,T)}\cdot\left[1 + 0.046263\cdot\left(\mathrm{Rerec6}(G,T)\cdot\frac{\mathrm{dcell6}}{z}\right)\right]^{0.45363}$$

Average coefficient of friction
for a smooth square channel

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta\mathrm{Prec8}_{\mathrm{jcase}+1} := 4\cdot \mathrm{cfricrec8}\left(\mathrm{Grec}_{\mathrm{jcase}+1},\mathrm{Tavg}_{\mathrm{jcase}+1},\mathrm{Lrec}\right)\cdot\frac{\frac{\left(\mathrm{Urec}_{\mathrm{jcase}+1}\right)^2}{2}\cdot\left[\rho\mathrm{mixrec}\left(\mathrm{Trecin}_{\mathrm{jcase}+1}\right) + \rho\mathrm{mixrec}\left(\mathrm{Trecout}_{\mathrm{jcase}+1}\right)\cdot\left(\frac{\mathrm{Trec}}{\mathrm{Trec}}\right.\right.}{2}$$

$$\Delta\mathrm{Prec6}_{\mathrm{jcase}+1} := 4\cdot \mathrm{cfricrec6}\left(\mathrm{Grec}_{\mathrm{jcase}+1},\mathrm{Tavg}_{\mathrm{jcase}+1},\mathrm{Lrec}\right)\cdot\frac{\frac{\left(\mathrm{Urec}_{\mathrm{jcase}+1}\right)^2}{2}\cdot\left[\rho\mathrm{mixrec}\left(\mathrm{Trecin}_{\mathrm{jcase}+1}\right) + \rho\mathrm{mixrec}\left(\mathrm{Trecout}_{\mathrm{jcase}+1}\right)\cdot\left(\frac{\mathrm{Trec}}{\mathrm{Trec}}\right.\right.}{2}$$

$$\frac{\Delta\mathrm{Prec8}}{\mathrm{Prec}} = \begin{bmatrix} 0 \\ 0.0097 \\ 0.013 \\ 0.0162 \\ 0.0203 \\ 0.0393 \end{bmatrix} \qquad \frac{\Delta\mathrm{Prec6}}{\mathrm{Prec}} = \begin{bmatrix} 0 \\ 0.0071 \\ 0.0095 \\ 0.0119 \\ 0.0149 \\ 0.0289 \end{bmatrix} \qquad \Delta\mathrm{Pobs\_P} := \begin{bmatrix} 0 \\ 0.011 \\ 0.014 \\ 0.018 \\ 0.022 \\ 0.042 \end{bmatrix}$$

Chose 800 cells per in2
with 10% length factor
in Lrec for chevrons

Averaged Nu for 800 cpi square channels (fully developed laminar flow) taken from Rosner:

$$Nuhavgrec8_{jcase+1} := 2.976 \cdot \left[1 + \left[\frac{7.6 \cdot (Lrec \cdot 1.1)}{Rerec8\left(Grec_{jcase+1}, Tavg_{jcase+1}\right) \cdot Pr\left(Tavg_{jcase+1}\right) \cdot dcell8} \right]^{\frac{8}{3}} \right]^{\frac{1}{8}}$$

$$Nuhavgrec8 = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.976 \\ 2.9762 \end{bmatrix}$$

Entrance effect for heat transfer within the recuperator is only significant for the first half inch - average Nusselt No. = 2.976 for all cases

$$hrecavg_{jcase+1} := \frac{\lambda mix\left(Tavg_{jcase+1}\right) \cdot Nuhavgrec8_{jcase+1}}{dcell8}$$

$$hrecavg = \begin{bmatrix} 0 \\ 188.0022 \\ 190.6356 \\ 193.2448 \\ 195.8307 \\ 197.1273 \end{bmatrix} \cdot kg \cdot sec^{-3} \cdot K^{-1}$$

W/m2/K

$$\Delta Tskin_{jcase+1} := \frac{Grec_{jcase+1} \cdot dcell8 \cdot \left(Cpmix\left(Trecout_{jcase+1}\right) \cdot Trecout_{jcase+1} - Cpmix\left(Trecin_{jcase+1}\right) \cdot Trecin_{jcase+1}\right)}{MWmix \cdot hrecavg_{jcase+1} \cdot 4 \cdot Lrec \cdot 1.1}$$

$$\Delta Tskin = \begin{bmatrix} 0 \\ -7.5657 \\ -9.274 \\ -10.5339 \\ -11.9549 \\ -13.635 \end{bmatrix} \cdot K \qquad \Delta Tskin \cdot 2 \cdot \frac{9}{5 \cdot K} = \begin{bmatrix} 0 \\ -27.2364 \\ -33.3864 \\ -37.9221 \\ -43.0378 \\ -49.0859 \end{bmatrix}$$

Approximate average ΔT (F) across wall in recuperator

ΔT seems low - more conservative calculation uses dcell for 600 cells/in2 - in this case ΔT maximum increases from 50F to about 70F

$$\Delta Tskin \cdot 2 \cdot \frac{9}{5 \cdot K} \cdot \left(\frac{dcell6}{dcell8}\right)^2 = \begin{bmatrix} 0 \\ -37.2231 \\ -45.628 \\ 51.8268 \\ -58.8182 \\ -67.0839 \end{bmatrix} \qquad \left(\frac{dcell6}{dcell8}\right)^2 = 1.3667$$

Use 600 cells/in2 in recuperator dimension for conservative calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavgrec6c1_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lrec\cdot 1.1}{Rerec6\left(Grec_{jcase+1},Tavg_{jcase+1}\right)\cdot Sc1T\left(Tavg_{jcase+1}\right)\cdot dcell6}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavgrec6c1 = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9765 \end{bmatrix}$$

$$Numavgrec6c7_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lrec\cdot 1.1}{Rerec6\left(Grec_{jcase+1},Tavg_{jcase+1}\right)\cdot Sc7T\left(Tavg_{jcase+1}\right)\cdot dcell6}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavgrec6c7 = \begin{bmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9775 \\ 2.9784 \\ 2.9891 \end{bmatrix}$$

$$Numavgrec6co_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lrec\cdot 1.1}{Rerec6\left(Grec_{jcase+1},Tavg_{jcase+1}\right)\cdot SccoT\left(Tavg_{jcase+1}\right)\cdot dcell6}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavgrec6co = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9766 \end{bmatrix}$$

Once again the entrance effects within the recuperator are negligible

The average (integral) Nusselt numbers at 1-atm show very little contribution of the thermal entry length, i.e. the flow velocities and heat and mass transfer coefficients have values close to those in long channels.

Now determine the maximum possible CH4, C7H14, and CO conversions in a 600 cells per in2 recuperator

$ych40 := 0.005 \qquad yc7h140 := 0.0005 \qquad yco0 := 0.005$

Start with maximum concentrations of added pollutants

$$ych4rec6_{jcase+1} := ych40\cdot\exp\left(\frac{-4\cdot Lrec\cdot 1.1\cdot Numavgrec6c1_{jcase+1}}{Rerec6\left(Grec_{jcase+1},Tavg_{jcase+1}\right)\cdot Sc1T\left(Tavg_{jcase+1}\right)\cdot dcell6}\right)$$

$$\frac{4\cdot Lrec\cdot 1.1\cdot Numavgrec6c1_{jcase+1}}{Rerec6\left(Grec_{jcase+1},Tavg_{jcase+1}\right)\cdot Sc1T\left(Tavg_{jcase+1}\right)\cdot dcell6} = \begin{array}{|c|} \hline 65.4083 \\ 50.9771 \\ 42.7552 \\ 35.7764 \\ 19.0017 \\ \hline \end{array} \qquad \frac{ych4rec6}{ych40} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 5.5932\cdot 10^{-9} \end{bmatrix}$$

$$yc7h14rec6_{jcase+1} = yc7h140 \cdot \exp\left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6\left(Grec_{jcase+1}, Tavg_{jcase+1}\right) \cdot Sc7T\left(Tavg_{jcase+1}\right) \cdot dcell6}\right)$$

$$yc7h14rec6 = \begin{bmatrix} 0 \\ 3.5287 \cdot 10^{-12} \\ 2.1834 \cdot 10^{-10} \\ 2.2859 \cdot 10^{-9} \\ 1.6805 \cdot 10^{-8} \\ 2.0597 \cdot 10^{-6} \end{bmatrix} \qquad \frac{yc7h14rec6}{yc7h140} = \begin{bmatrix} 0 \\ 7.057 \cdot 10^{-9} \\ 4.367 \cdot 10^{-7} \\ 4.572 \cdot 10^{-6} \\ 3.361 \cdot 10^{-5} \\ 4.119 \cdot 10^{-3} \end{bmatrix}$$

$$\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6c7_{jcase+1}}{Rerec6\left(Grec_{jcase+1}, Tavg_{jcase+1}\right) \cdot Sc7T\left(Tavg_{jcase+1}\right) \cdot dcell6}$$

-18.7692
-14.6441
-12.2956
-10.3007
-5.492

$$ycorec6_{jcase+1} = yco0 \cdot \exp\left(\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6\left(Grec_{jcase+1}, Tavg_{jcase+1}\right) \cdot SccoT\left(Tavg_{jcase+1}\right) \cdot dcell6}\right)$$

$$ycorec6 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1.457 \cdot 10^{-10} \end{bmatrix} \qquad \frac{ycorec6}{yco0} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 6.4676 \cdot 10^{-15} \\ 2.914 \cdot 10^{-8} \end{bmatrix}$$

$$\frac{-4 \cdot Lrec \cdot 1.1 \cdot Numavgrec6co_{jcase+1}}{Rerec6\left(Grec_{jcase+1}, Tavg_{jcase+1}\right) \cdot SccoT\left(Tavg_{jcase+1}\right) \cdot dcell6}$$

-59.7854
-46.5803
-39.0561
-32.672
-17.3512

With 5000ppm C7H14 in turbine exhaust, exit concentration reaches 20 ppm at the highest power level for conservative 600 cells/in2 calculation. For 800 cells/in2, the exit concentration in this case would reach about 2 ppm. With only 500ppm C7H14 in the inlet, should get <2 ppm in the outlet of the recuperator assuming favorable catalytic rates at the wall. Also this calculation used averaged temperature and flow conditions - will compare below a 1-dimensional (axial) calculation that determines the effect of decreasing temperature on the kinetics and mass transport.

Maximum possible (transport-limited) CO and CH4 conversions in a 7 in. 600-800 cells/in2 recuperator are >99.99%, while cyclohexane conversion is >99.6%. The final CO and C7H14 levels are < 1 ppb and .2 ppm for post turbine concentrations of 1000 and 50 ppm, respectively.

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An alternative method of calculating performance uses local Nusselt numbers for heat and mass transfer to determine the wall temperature and combustion rates at the wall. First we define the local Nu function then check conversion assuming fast kinetics and compare with the previous averaged (integrated) Nu formula.

Local Nu(x) taken from Kays & Crawford for hydro & thermal laminar flow entrance with circular channel (modified for square channel by a factor 2.96/3.66:

$ncase := 5$

$Numono(z) := (1 + \exp(-1.09689 - 0.381402 \cdot \ln(z) - 8.287774 \cdot z^{0.5})) \cdot 2.976 \qquad Numono(0.1152163) = 3.112$

$$zzchar6c7_{jcase+1} := \frac{Rerec6(Grec_{jcase+1}, Trecin_{jcase+1}) \cdot Sc7T(Trecin_{jcase+1}) \cdot dcell6}{2} \qquad \frac{Lrec}{zzchar6c7_{ncase}} = 0.9444$$

Case specific

$$zzchar6c1_{jcase+1} := \frac{Rerec6(Grec_{jcase+1}, Trecin_{jcase+1}) \cdot Sc1T(Trecin_{jcase+1}) \cdot dcell6}{2} \qquad \frac{Lrec}{zzchar6c1_{ncase}} = 3.2574$$

Case specific

$nz := 400$

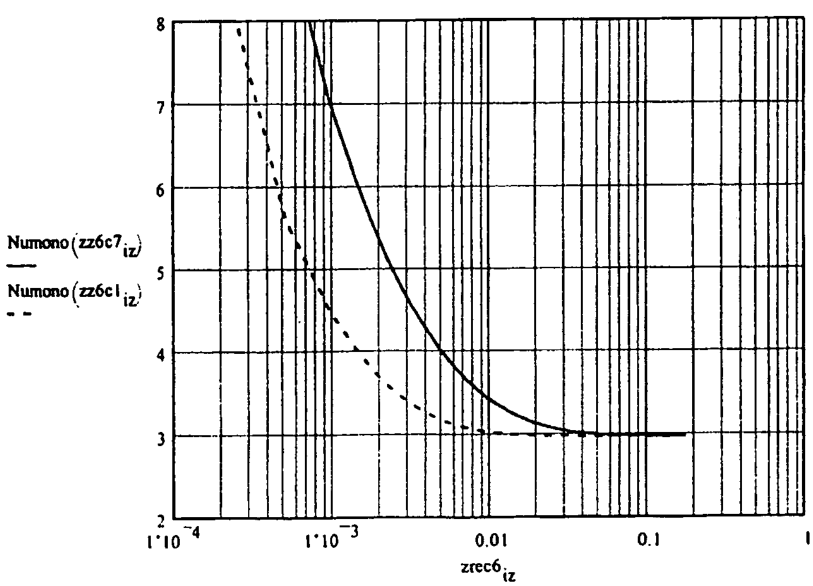
$iz := 0 .. nz$

$Lrec = 17.78 \cdot cm \qquad dcell6 = 0.0961 \cdot cm$

$$zrec6_{iz} := iz \cdot \frac{Lrec}{nz} + dwall6 \qquad zz6c7_{iz} := \frac{zrec6_{iz}}{zzchar6c7_{ncase}} \quad zz6c1_{iz} := \frac{zrec6_{iz}}{zzchar6c1_{ncase}}$$

$$zzchar6c7 = \begin{bmatrix} 0 \\ 4.896 \\ 6.3647 \\ 7.6867 \\ 9.3023 \\ 18.8265 \end{bmatrix} \cdot cm$$

$$zzchar6c1 = \begin{bmatrix} 0 \\ 1.4244 \\ 1.8518 \\ 2.2364 \\ 2.7064 \\ 5.4583 \end{bmatrix} \cdot cm$$



Case specific $ncase = 5$

Case specific ncase = 5

$$kgpbl6c7(T,z) := \frac{Dc7h14T(T)\cdot Numono\left(\frac{z}{zzchar6c7_{ncase}}\right)}{dcell6}$$

$kgpbl6c7(Trecin_{ncase}, Lrec) = 13.6159\cdot sec^{-1}\cdot cm$

$$kgpbl6c1(T,z) := \frac{Dch4T(T)\cdot Numono\left(\frac{z}{zzchar6c1_{ncase}}\right)}{dcell6}$$

$kgpbl6c1(Trecin_{ncase}, Lrec) = 46.9581\cdot sec^{-1}\cdot cm$

$$Trecz_{iz} := Trecin_{ncase} - \frac{Trecin_{ncase} - Trecout_{ncase}}{nz}\cdot iz$$

$Trecz_{nz} = 630.3722\cdot K$ $\quad Trecout_{ncase} = 630.3722\cdot K$

****

Determine maximum conversion of fuels with very fast catalytic combustion rates (zero fuel concentration at the wall)

ncase = 5

$yzc7h14_0 := yc7h140$ $\quad yzch4_0 := ych40$

$$yzc7h14_{iz+1} := \left(1 - kgpbl6c7(Trecz_{iz}, zrec6_{iz})\cdot\frac{Lrec}{nz}\cdot 1.1\cdot\frac{4}{dcell6}\cdot\frac{\varepsilon cell6}{Urec_{ncase}}\cdot\frac{Trecin_{ncase}}{Trecz_{iz}}\right)\cdot yzc7h14_{iz}$$

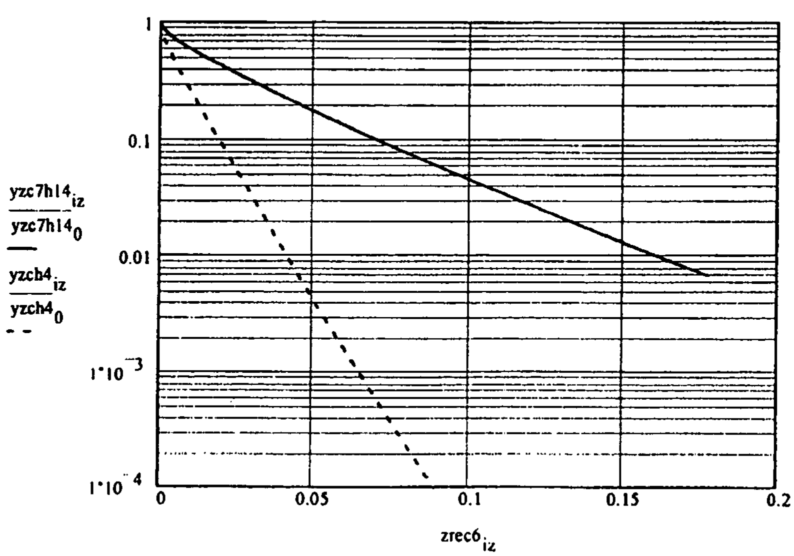
Case specific

$$yzch4_{iz+1} := \left(1 - kgpbl6c1(Trecz_{iz}, zrec6_{iz})\cdot\frac{Lrec}{nz}\cdot 1.1\cdot\frac{4}{dcell6}\cdot\frac{\varepsilon cell6}{Urec_{ncase}}\cdot\frac{Trecin_{ncase}}{Trecz_{iz}}\right)\cdot yzch4_{iz}$$

Case specific

$yzc7h14_{nz} = 3.385\cdot 10^{-6}$ $\quad yzc7h14_0 = 0.0005$ $\quad \frac{yzc7h14_{nz}}{yzc7h14_0} = 6.77\cdot 10^{-3}$ $\quad \frac{yzch4_{nz}}{yzch4_0} = 4.3292\cdot 10^{-8}$

$yzch4_{nz} = 2.1646\cdot 10^{-10}$ $\quad yzch4_0 = 0.005$



Conversion of C7H14 under case 5 (full power) is 99.3% [vs. 99.6% via averaged integrated formulas] with about 1 inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within 3.5 inches.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

Case specific ncase = 5

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Add finite rate kinetics for PdO/Al2O3 methane combustion catalyst
Begin by defining a few constants and catalyst functions

$R = 82.076 \cdot K^{-1} \cdot atm \cdot cm^3$ atm*cm3/mol*K

$Rcm := 83143000 \cdot gm \cdot cm^2 \cdot sec^{-2} \cdot K^{-1}$ $TOL := 0.0001$

Define Catalyst Functions:

$$\eta sph(\phi) := \frac{3}{\phi} \cdot \left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi} \right)$$

$$\eta fpl(\phi) := \frac{\tanh(\phi)}{\phi}$$

Catalyst Physical Properties for Pd/Al2O3

$Scat := 85 \cdot m^2 \cdot gm^{-1}$ $\rho catpart := 2.5 \cdot gm \cdot cm^{-3}$

$V\mu pore := 0.15 \cdot cm^3 \cdot gm^{-1}$ $dpcat := 0.0002 \cdot cm$

$Lcat := 0.0020 \cdot cm$

$d\mu pore := 6 \cdot \frac{V\mu pore}{Scat}$ $\varepsilon\mu pore := 0.375$ $\tau\mu pore := 3.0$

$d\mu pore = 1.0588 \cdot 10^{-6} \cdot cm$

****

$$DeffCH4(T) := \frac{\dfrac{\varepsilon\mu pore}{\tau\mu pore}}{\left(\dfrac{1}{Dch4T(T)} + \dfrac{3}{d\mu pore \cdot \sqrt{\dfrac{\frac{8}{\pi} \cdot R \cdot T}{MW_0}}} \right)}$$

$$d\mu pore \cdot \sqrt{\frac{\frac{8}{\pi} \cdot R \cdot Tin}{MW_0}} = 0.1095 \cdot sec^{-1} \cdot cm^2$$

$DeffCH4(Tin) = 4.43271 \cdot 10^{-3} \cdot sec^{-1} \cdot cm^2$ $Dch4T(Tin) = 1.2343 \cdot sec^{-1} \cdot cm^2$

$$\mathrm{DeffC7H14}(T) := \frac{\dfrac{\varepsilon\mu\mathrm{pore}}{\tau\mu\mathrm{pore}}}{\left[\dfrac{1}{\mathrm{Dc7h14T}(T)} + \dfrac{3}{d\mu\mathrm{pore}\cdot\sqrt{\dfrac{\frac{8}{\pi}\cdot R\cdot T}{MW_6}}}\right]}$$

$$d\mu\mathrm{pore}\cdot\sqrt{\frac{\frac{8}{\pi}\cdot R\cdot \mathrm{Tin}}{MW_6}} = 0.0829\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}^2$$

$$\mathrm{DeffC7H14}(\mathrm{Tin}) = 3.20528\cdot 10^{-3}\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}^2 \qquad \mathrm{Dc7h14}(\mathrm{Tin}) = 0.356\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}^2$$

$$\mathrm{DmacCH4}(T) := \frac{0.4}{2.5}\cdot \mathrm{Dch4T}(T) \qquad \mathrm{DmacCH4}(800\cdot K) = 0.193\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}^2$$

$$\mathrm{DmacC7H14}(T) := \frac{0.4}{2.5}\cdot \mathrm{Dc7h14T}(T) \qquad \mathrm{DmacC7H14}(800\cdot K) = 0.0556\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}^2$$

$$\mathrm{k0T} := 1.0\cdot \mathrm{gm}^{-1}\cdot \mathrm{sec}^{-1}$$

Test value for k0T

Microscopic Thiele Modulus for CH4

$$\phi\mu(k,T) := \sqrt{\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot\frac{k}{\mathrm{DeffCH4}(T)}\right]}\cdot\frac{\mathrm{dpcat}}{6} \qquad \phi\mu(\mathrm{k0T},\mathrm{Tin}) = 0.2042$$

Macroscopic Thiele Modulus for CH4

$$\Phi\mathrm{mac}(k,T) := \sqrt{\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot k\right]\cdot\frac{\eta\mathrm{sph}(\phi\mu(k,T))}{\mathrm{DmacCH4}(T)}}\cdot \mathrm{Lcat} \qquad \Phi\mathrm{mac}(\mathrm{k0T},\mathrm{Tin}) = 1.8333$$

Microscopic Thiele Modulus for C7H14

$$\phi\mu7(k,T) := \sqrt{\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot\frac{k}{\mathrm{DeffC7H14}(T)}\right]}\cdot\frac{\mathrm{dpcat}}{6} \qquad \phi\mu7(\mathrm{k0T},\mathrm{Tin}) = 0.2402$$

Macroscopic Thiele Modulus for C7H14

$$\Phi\mathrm{mac7}(k,T) := \sqrt{\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot k\right]\cdot\frac{\eta\mathrm{sph}(\phi\mu7(k,T))}{\mathrm{DmacC7H14}(T)}}\cdot \mathrm{Lcat} \qquad \Phi\mathrm{mac7}(\mathrm{k0T},\mathrm{Tin}) = 3.4117$$

$$\mathrm{RatekCH4}(k,T) := \eta\mathrm{sph}(\phi\mu(k,T))\cdot\eta\mathrm{fpl}(\Phi\mathrm{mac}(k,T))\cdot\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot k\right] \qquad \mathrm{RatekCH4}(\mathrm{k0T},\mathrm{Tin}) = 85999.4914\cdot \mathrm{sec}^{-1}$$

$$\mathrm{RatekC7H14}(k,T) := \eta\mathrm{sph}(\phi\mu7(k,T))\cdot\eta\mathrm{fpl}(\Phi\mathrm{mac7}(k,T))\cdot\left[\rho\mathrm{catpart}\cdot\left(\frac{R\cdot T}{\mathrm{Pref}}\right)\cdot k\right] \qquad \mathrm{RatekC7H14}(\mathrm{k0T},\mathrm{Tin}) = 48479.296\cdot \mathrm{sec}^{-1}$$

****

Defines transport restricted rate constant function given catalyst effective first order rate constant, k0T, methane or cyclohexane concentration, x, and surface temperature, T

PdO Catalyst Rate Constants

$Erpd0 := 12800 \cdot K \qquad Erpd1 := 4900 \cdot K \qquad Erpd3 := 15000 \cdot K$

Region0 - low T PdO to 625K ignores inhibition by H2O and CO2	Region1 - Intermediate T 625K to 909K	Region2 - Flat 909K to 1048K decomposition	Region3 - Pd metal

$$Apd0 := 2.4 \cdot 10^3 \cdot 200 \cdot gm^{-1} \cdot sec^{-1} \qquad Apd1 := Apd0 \cdot \exp\left(-\frac{Erpd0}{625 \cdot K} + \frac{Erpd1}{625 \cdot K}\right)$$

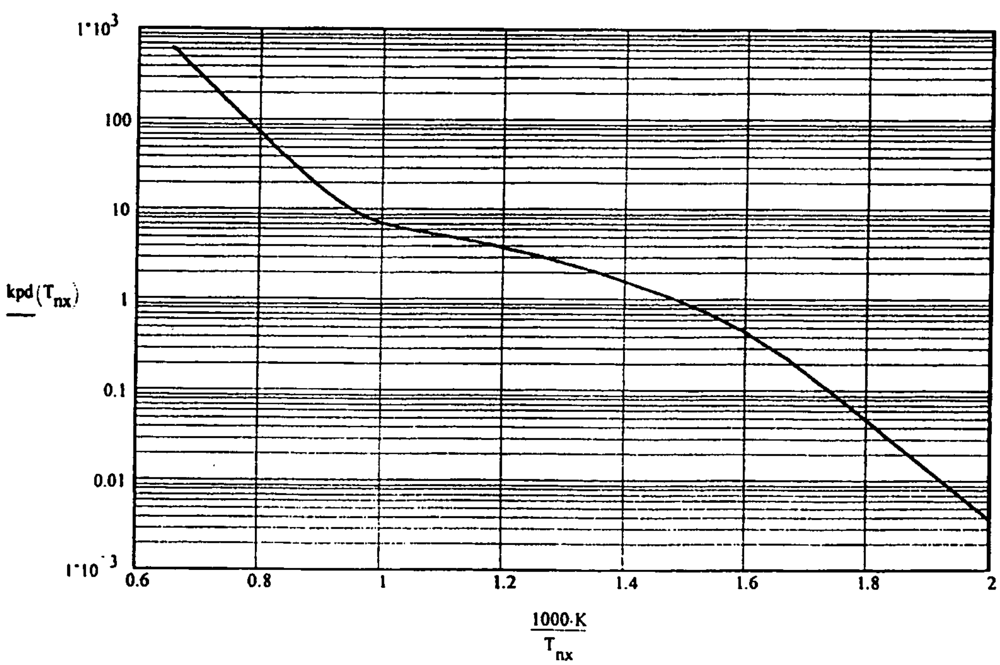
$$Apd2 := Apd1 \cdot \exp\left(\frac{-Erpd1}{909.1 \cdot K}\right) \qquad Apd3 := Apd2 \cdot \exp\left(\frac{Erpd3}{1048.1 \cdot K}\right)$$

Interpolation formula for the four PdO+Pd rate constants

$$kpd(T) := \left[Apd3^2 \cdot \exp\left(-\frac{2 \cdot Erpd3}{T}\right) + \frac{1}{\left(Apd2^{-2} + Apd1^{-2} \cdot \exp\left(\frac{2 \cdot Erpd1}{T}\right) + Apd0^{-2} \cdot \exp\left(\frac{2 \cdot Erpd0}{T}\right)\right)} \right]^{0.5}$$

$nx := 0, 1 .. 41 \qquad T_{nx} := 500 \cdot K + nx \cdot 25 \cdot K$

CATALYTIC RATE CONSTANT vs TEMPERATURE (mol/atmCH4/s/gcat)



$$\mathrm{keffrec6c1}(T,z) := \frac{1}{\left(\frac{1}{\mathrm{RatekCH4}(\mathrm{kpd}(T),T)\cdot \mathrm{Lcat}}\right)+\frac{1}{\mathrm{kgpbl6c1}(T,z)}}$$

$\mathrm{kgpbl6c1}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 35.3023\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$

$\mathrm{keffrec6c1}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 0.7922\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$

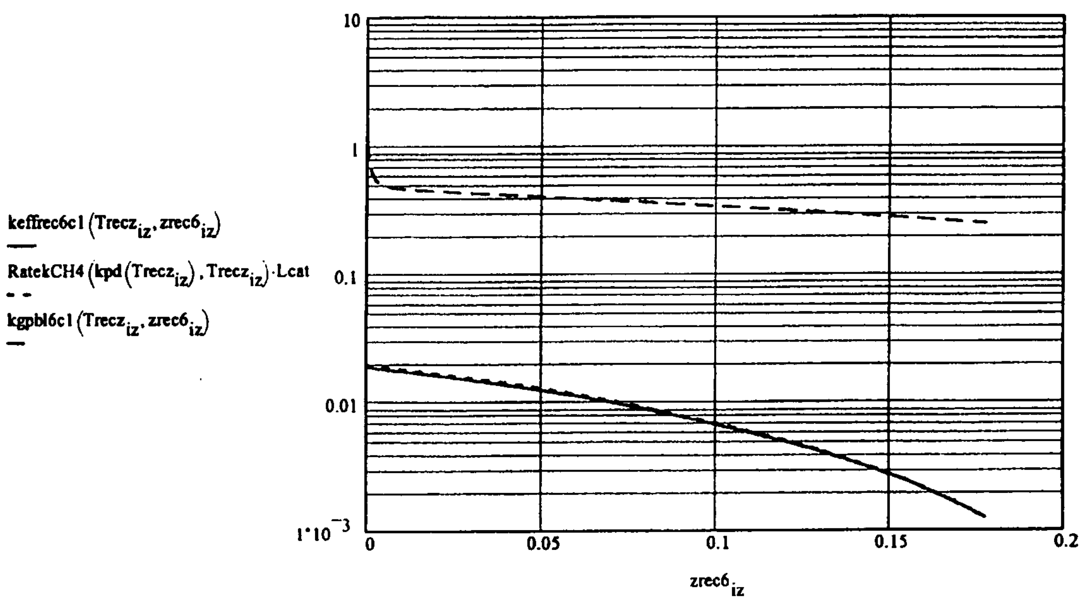
$\mathrm{RatekCH4}\left(\mathrm{kpd}\left(\mathrm{Tavg}_{\mathrm{ncase}}\right),\mathrm{Tavg}_{\mathrm{ncase}}\right)\cdot \mathrm{Lcat} = 0.8104\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$

$$\mathrm{keffrec6c7}(T,z) := \frac{1}{\left(\frac{1}{\mathrm{RatekC7H14}(10\cdot \mathrm{kpd}(T),T)\cdot \mathrm{Lcat}}\right)+\frac{1}{\mathrm{kgpbl6c7}(T,z)}}$$

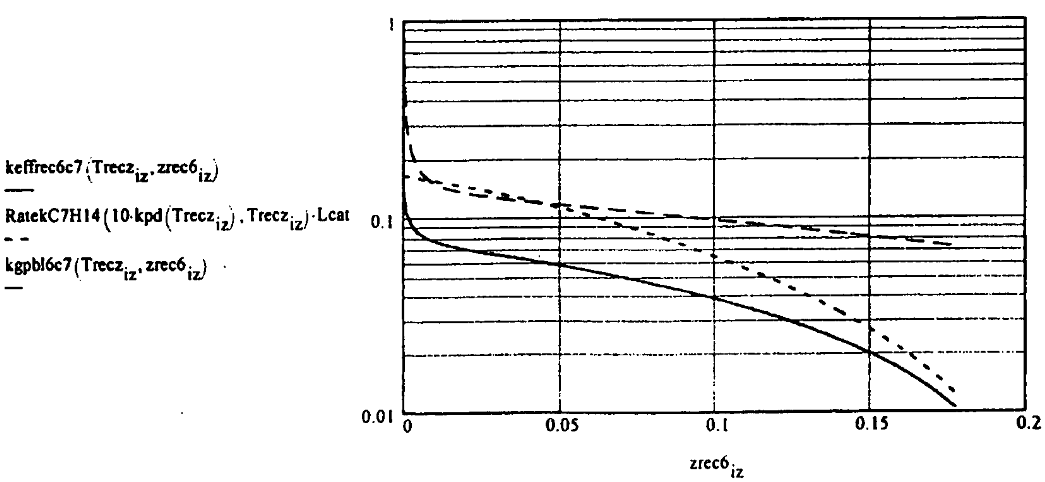
$\mathrm{kgpbl6c7}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 10.1756\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$

$\mathrm{keffrec6c7}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 4.2778\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$

$\mathrm{RatekC7H14}\left(10\cdot \mathrm{kpd}\left(\mathrm{Tavg}_{\mathrm{ncase}}\right),\mathrm{Tavg}_{\mathrm{ncase}}\right)\cdot \mathrm{Lcat} = 7.3807\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$



Case specific $\mathrm{ncase} = 5$



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Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $ncase = 5$

$$Trecz_{iz} := Trecin_{ncase} - \frac{Trecin_{ncase} - Trecout_{ncase}}{nz} \cdot iz \qquad Trecz_{nz} = 630.3722 \cdot K \qquad Trecout_{ncase} = 630.3722 \cdot K$$

$$yzkc7h14_0 := yc7h140 \qquad yzkch4_0 := ych40$$

$$yzkc7h14_{iz+1} := \left(1 - keffrec6c7\left(Trecz_{iz}, zrec6_{iz}\right) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}}\right) \cdot yzkc7h14_{iz}$$

Case specific

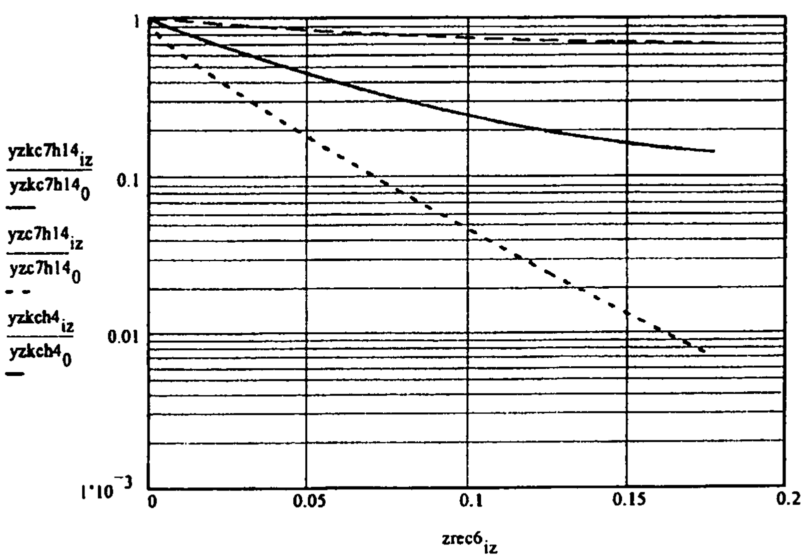
$ncase = 5$

$$yzkch4_{iz+1} := \left(1 - keffrec6c1\left(Trecz_{iz}, zrec6_{iz}\right) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}}\right) \cdot yzkch4_{iz}$$

Case specific

$$yzkc7h14_{nz} = 7.036 \cdot 10^{-5} \qquad yzkc7h14_0 = 0.0005 \qquad \frac{yzkc7h14_{nz}}{yzkc7h14_0} = 1.407 \cdot 10^{-1} \qquad \frac{yzkch4_{nz}}{yzkch4_0} = 0.6838$$

$$yzkch4_{nz} = 0.0034 \qquad yzkch4_0 = 0.005$$



Case specific $ncase = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.3% for the maximum BL transport-limited conversion] with gradually decreasing (rate limited) conversion. Conversion of CH4 is very poor (35%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.

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In the following section, the conversion of C7H14, CH4 and CO is considered for various honeycomb monliths

****

$$Thc_{jcase+1} := Trecin_{jcase+1} \qquad \rho mixhc_{jcase+1} := \rho mixrec\left(Trecin_{jcase+1}\right)$$

$$Ghc2_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell2} \qquad Ghc4_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell4} \qquad Ghc6_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1} \qquad Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1} \qquad Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} := \frac{Ghc2_{jcase+1} \cdot dcell2}{\mu mixT\left(Thc_{jcase+1}\right)} \qquad Rehc4_{jcase+1} := \frac{Ghc4_{jcase+1} \cdot dcell4}{\mu mixT\left(Thc_{jcase+1}\right)} \qquad Rehc6_{jcase+1} := \frac{Ghc6_{jcase+1} \cdot dcell6}{\mu mixT\left(Thc_{jcase+1}\right)}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix} \qquad Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix} \qquad Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrichc2(j,z) := \frac{14.227}{Rehc2_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{dcell2}{z}\right)\right]^{0.45363}$$

$$cfrichc4(j,z) := \frac{14.227}{Rehc4_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{dcell4}{z}\right)\right]^{0.45363}$$

Average coefficients of friction for smooth square channels

$$cfrichc6(j,z) := \frac{14.227}{Rehc6_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{dcell6}{z}\right)\right]^{0.45363}$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta Phc2_{jcase+1} := 4\cdot cfrichc2(jcase+1, Lhc)\cdot\frac{\left(Uhc2_{jcase+1}\right)^2}{2}\cdot\rho mixhc_{jcase+1}\cdot\frac{Lhc}{dcell2}$$

$$\Delta Phc4_{jcase+1} := 4\cdot cfrichc4(jcase+1, Lhc)\cdot\frac{\left(Uhc4_{jcase+1}\right)^2}{2}\cdot\rho mixhc_{jcase+1}\cdot\frac{Lhc}{dcell4}$$

$$\Delta Phc6_{jcase+1} := 4\cdot cfrichc6(jcase+1, Lhc)\cdot\frac{\left(Uhc6_{jcase+1}\right)^2}{2}\cdot\rho mixhc_{jcase+1}\cdot\frac{Lhc}{dcell6}$$

$$\frac{\Delta Phc2}{Phc} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix} \qquad \frac{\Delta Phc4}{Phc} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix} \qquad \frac{\Delta Phc6}{Phc} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix} \qquad \Delta Phcmax\_P := \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 400 cells per in2 honeycombs via estimated ΔP

****

Use 400 cells/in2 in honeycomb monolith for calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavghc4cl_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lhc}{Rehc4_{jcase+1}\cdot Sc1T\left(Thc_{jcase+1}\right)\cdot dcell4}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavghc4cl = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9762 \\ 2.9774 \end{bmatrix}$$

$$Numavghc4co_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lhc}{Rehc4_{jcase+1}\cdot SccoT\left(Thc_{jcase+1}\right)\cdot dcell4}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavghc4co = \begin{bmatrix} 0 \\ 2.976 \\ 2.9761 \\ 2.9762 \\ 2.9763 \\ 2.9778 \end{bmatrix}$$

****

$$Numavghc4c7_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lhc}{Rehc4_{jcase+1}\cdot Sc7T\left(Thc_{jcase+1}\right)\cdot dcell4}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}}$$

$$Numavghc4c7 = \begin{bmatrix} 0 \\ 2.977 \\ 2.9781 \\ 2.9795 \\ 2.9817 \\ 3.0123 \end{bmatrix}$$

Once again the entrance effects within monoliths are generally small

****

Now determine the maximum possible CH4, C7H14, and CO conversions in a 400 cells per in2 monolith

$ych40 := 0.005$ $\qquad$ $yc7h140 := 0.0005$ $\qquad$ $yco0 := 0.005$

$$ych4hc4_{jcase+1} := ych40\cdot \exp\left(\frac{-4\cdot Lhc\cdot Numavghc4c1_{jcase+1}}{Rehc4_{jcase+1}\cdot Sc1T\left(Thc_{jcase+1}\right)\cdot dcell4}\right)$$

$$\frac{-4\cdot Lhc\cdot Numavghc4c1_{jcase+1}}{Rehc4_{jcase+1}\cdot Sc1T\left(Thc_{jcase+1}\right)\cdot dcell4}$$

-48.7678
-37.5142
-31.0633
-25.6688
-12.7326

$$\frac{ych4hc4}{ych40} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3.2315\cdot 10^{-14} \\ 7.1151\cdot 10^{-12} \\ 2.9532\cdot 10^{-6} \end{bmatrix}$$

$$ycohc4_{jcase+1} := yco0\cdot \exp\left(\frac{-4\cdot Lhc\cdot Numavghc4co_{jcase+1}}{Rehc4_{jcase+1}\cdot SccoT\left(Thc_{jcase+1}\right)\cdot dcell4}\right)$$

$$\frac{ycohc4}{yco0} = \begin{bmatrix} 0 \\ 0 \\ 1.4726\cdot 10^{-15} \\ 5.2301\cdot 10^{-13} \\ 7.0997\cdot 10^{-11} \\ 9.1398\cdot 10^{-6} \end{bmatrix}$$

$$\frac{-4\cdot Lhc\cdot Numavghc4co_{jcase+1}}{Rehc4_{jcase+1}\cdot SccoT\left(Thc_{jcase+1}\right)\cdot dcell4}$$

-44.3966
-34.1518
-28.2792
-23.3684
-11.6029

$$yc7h14hc4_{jcase+1} := yc7h140 \cdot \exp\left(\frac{-4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell4}\right) \qquad \frac{-4 \cdot Lhc \cdot Numavghc4c7_{jcase+1}}{Rehc4_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell4} = \begin{array}{|c|}\hline -14.1935 \\ \hline -10.9219 \\ \hline -9.0478 \\ \hline -7.482 \\ \hline -3.7348 \\ \hline \end{array}$$

$$\frac{yc7h14hc4}{yc7h140} = \begin{bmatrix} 0 \\ 6.8527 \cdot 10^{-7} \\ 1.8058 \cdot 10^{-5} \\ 0.0001 \\ 0.0006 \\ 0.0239 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (97.6%) fall below 99.9% with a 400 cells/in2 monolith. With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 1.2 ppm.

****

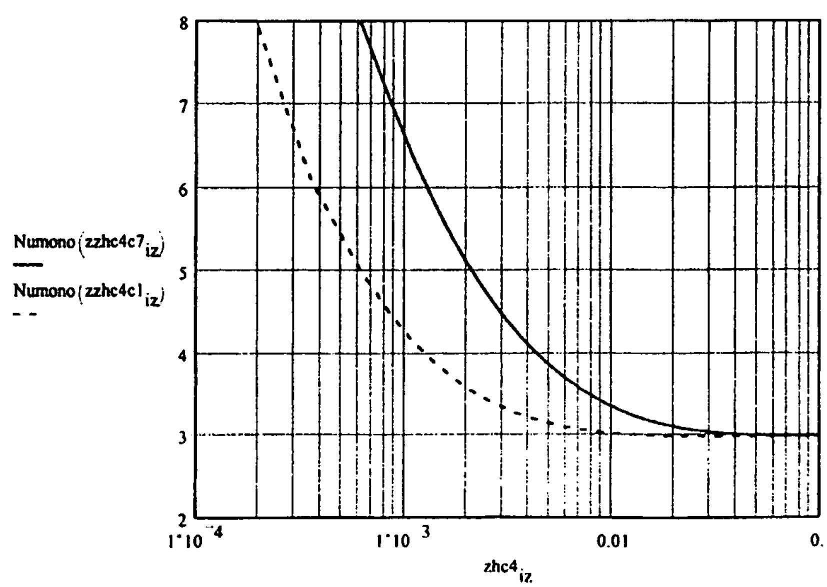
For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: $mcase := 5$

$$zzcharhc4c7_{jcase+1} := \frac{Rehc4_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell4}{2} \qquad \frac{Lhc}{zzcharhc4c7_{mcase}} = 0.6199$$

$$zzcharhc4c1_{jcase+1} := \frac{Rehc4_{jcase+1} \cdot Sc1T\left(Trecin_{jcase+1}\right) \cdot dcell4}{2} \qquad \frac{Lhc}{zzcharhc4c1_{mcase}} = 2.1382$$

$nz = 400 \qquad Lhc = 10.16 \cdot cm \qquad dcell4 = 0.1168 \cdot cm$

$$zhc4_{iz} := iz \cdot \frac{Lhc}{nz} + dwall4 \qquad zzhc4c7_{iz} := \frac{zhc4_{iz}}{zzcharhc4c7_{mcase}} \qquad zzhc4c1_{iz} := \frac{zhc4_{iz}}{zzcharhc4c1_{mcase}} \qquad zzcharhc4c7 = \begin{bmatrix} 0 \\ 4.2621 \\ 5.5407 \\ 6.6914 \\ 8.0979 \\ 16.389 \end{bmatrix} \cdot cm$$



Case specific mcase = 5

$$\text{kgpblhc4c7}(T,z) := \frac{\text{Dc7h14T}(T)\cdot\text{Numono}\left(\frac{z}{\text{zzcharhc4c7}_{\text{mcase}}}\right)}{\text{dcell4}}$$

$\text{kgpblhc4c7}\left(\text{Thc}_{\text{mcase}},\text{Lhc}\right) = 11.2014\cdot\text{sec}^{-1}\cdot\text{cm}$

$$\text{kgpblhc4c1}(T,z) := \frac{\text{Dch4T}(T)\cdot\text{Numono}\left(\frac{z}{\text{zzcharhc4c1}_{\text{mcase}}}\right)}{\text{dcell4}}$$

$\text{kgpblhc4c1}\left(\text{Thc}_{\text{mcase}},\text{Lhc}\right) = 38.6127\cdot\text{sec}^{-1}\cdot\text{cm}$

$$\text{keffhc4c1}(T,z) := \frac{1}{\left(\frac{1}{\text{RatekCH4}(\text{kpd}(T),T)\cdot\text{Lcat}}\right)+\frac{1}{\text{kgpblhc4c1}(T,z)}}$$

$\text{kgpblhc4c1}\left(\text{Thc}_{\text{mcase}},\frac{\text{Lhc}}{2}\right) = 38.615\cdot\text{sec}^{-1}\cdot\text{cm}$

$\text{keffhc4c1}\left(\text{Thc}_{\text{mcase}},\frac{\text{Lrec}}{2}\right) = 1.8533\cdot\text{sec}^{-1}\cdot\text{cm}$

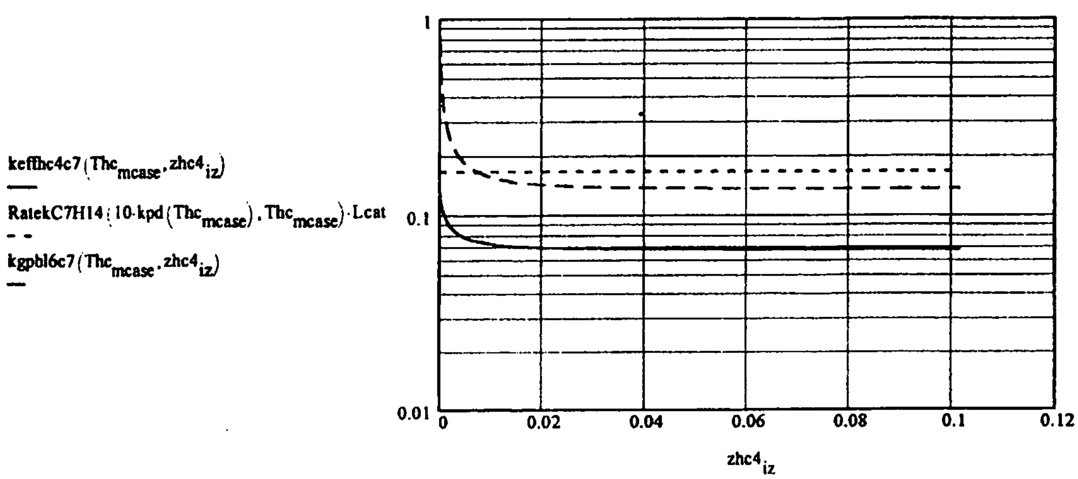
$\text{RatekCH4}\left(\text{kpd}\left(\text{Thc}_{\text{mcase}}\right),\text{Thc}_{\text{mcase}}\right)\cdot\text{Lcat} = 1.9467\cdot\text{sec}^{-1}\cdot\text{cm}$

$$\text{keffhc4c7}(T,z) := \frac{1}{\left(\frac{1}{\text{RatekC7H14}(10\cdot\text{kpd}(T),T)\cdot\text{Lcat}}\right)+\frac{1}{\text{kgpblhc4c7}(T,z)}}$$

$\text{kgpblhc4c7}\left(\text{Thc}_{\text{mcase}},\frac{\text{Lhc}}{2}\right) = 11.2528\cdot\text{sec}^{-1}\cdot\text{cm}$

$\text{keffhc4c7}\left(\text{Thc}_{\text{mcase}},\frac{\text{Lhc}}{2}\right) = 6.7062\cdot\text{sec}^{-1}\cdot\text{cm}$

$\text{RatekC7H14}\left(10\cdot\text{kpd}\left(\text{Thc}_{\text{mcase}}\right),\text{Thc}_{\text{mcase}}\right)\cdot\text{Lcat} = 16.5977\cdot\text{sec}^{-1}\cdot\text{cm}$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $mcase = 5$

$yzkhc4c7h14_0 := yc7h140$ $yzkhc4ch4_0 := ych40$

$$Thc = \begin{bmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{bmatrix} \cdot K$$

$$yzkhc4c7h14_{iz+1} := \left(1 - keffhc4c7\left(Thc_{mcase}, zhc4_{iz}\right)\cdot\frac{Lhc}{nz}\cdot\frac{4}{dcell4}\cdot\frac{\varepsilon cell4}{Uhc4_{mcase}}\right)\cdot yzkhc4c7h14_{iz}$$

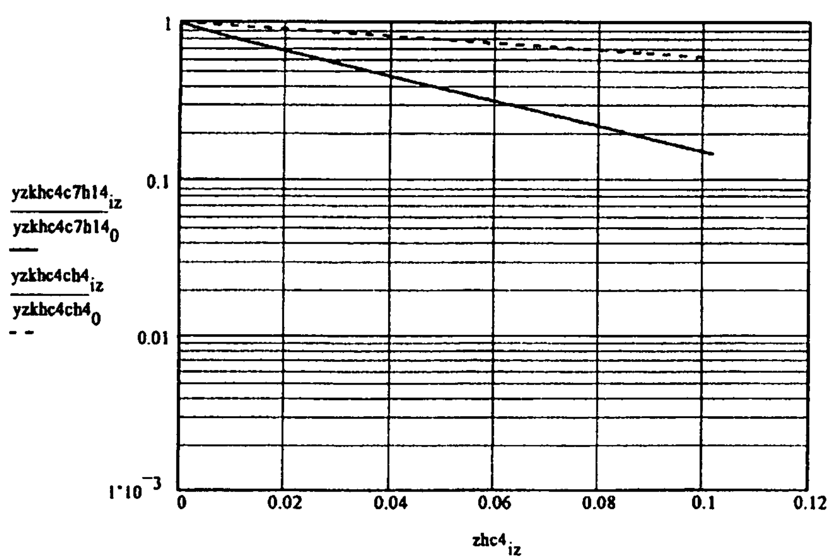
$$yzkhc4ch4_{iz+1} := \left(1 - keffhc4c1\left(Thc_{mcase}, zhc4_{iz}\right)\cdot\frac{Lhc}{nz}\cdot\frac{4}{dcell4}\cdot\frac{\varepsilon cell4}{Uhc4_{mcase}}\right)\cdot yzkhc4ch4_{iz}$$

Case specific

$mcase = 5$

$yzkhc4c7h14_{nz} = 7.281\cdot 10^{-5}$ $yzkhc4c7h14_0 = 0.0005$

$yzkhc4ch4_{nz} = 0.003$ $yzkhc4ch4_0 = 0.005$ $\dfrac{yzkhc4c7h14_{nz}}{yzkhc4c7h14_0} = 1.456\cdot 10^{-1}$ $\dfrac{yzkhc4ch4_{nz}}{yzkhc4ch4_0} = 0.5959$



Case specific $mcase = 5$

Conversion of C7H14 under case 5 (full power) is 99.4% [vs. 99.6% via averaged integrated formulas] with about 1-inch entry length. Conversion of CH4 (and also CO) is very high (>99.99%) within about 3.5-inch.

This result shows that the averaged integrated values for CH4, C7H14, and CO conversions are very good approximations and can be used for different values of fuel and CO concentrations.

Defines transport restricted rate constant function given catalyst effective first order rate constant, k0T, methane or cyclohexane concentration, x, and surface temperature, T

PdO Catalyst Rate Constants

$Erpd0 := 12800 \cdot K \qquad Erpd1 := 4900 \cdot K \qquad Erpd3 := 15000 \cdot K$

Region0 - low T PdO to 625K ignores inhibition by H2O and CO2 | **Region1 - Intermediate T 625K to 909K** | **Region2 - Flat 909K to 1048K decomposition** | **Region3 - Pd metal**

$Apd0 := 2.4 \cdot 10^{3} \cdot 200 \cdot gm^{-1} \cdot sec^{-1}$ $\qquad Apd1 := Apd0 \cdot \exp\left(-\frac{Erpd0}{625 \cdot K} + \frac{Erpd1}{625 \cdot K}\right)$ $\qquad Apd2 := Apd1 \cdot \exp\left(\frac{-Erpd1}{909.1 \cdot K}\right)$

$Apd3 := Apd2 \cdot \exp\left(\frac{Erpd3}{1048.1 \cdot K}\right)$

Interpolation formula for the four PdO+Pd rate constants

$$kpd(T) := \left[Apd3^{2} \cdot \exp\left(-\frac{2 \cdot Erpd3}{T}\right) + \frac{1}{\left(Apd2^{-2} + Apd1^{-2} \cdot \exp\left(\frac{2 \cdot Erpd1}{T}\right) + Apd0^{-2} \cdot \exp\left(\frac{2 \cdot Erpd0}{T}\right)\right)}\right]^{0.5}$$

Add expression for Pt(.5%)Pd(3.0%) catalyst with C3H8 here, use x2 for estimated rate constant with C7H14:

Rate constant via crushed powder results for C3H8

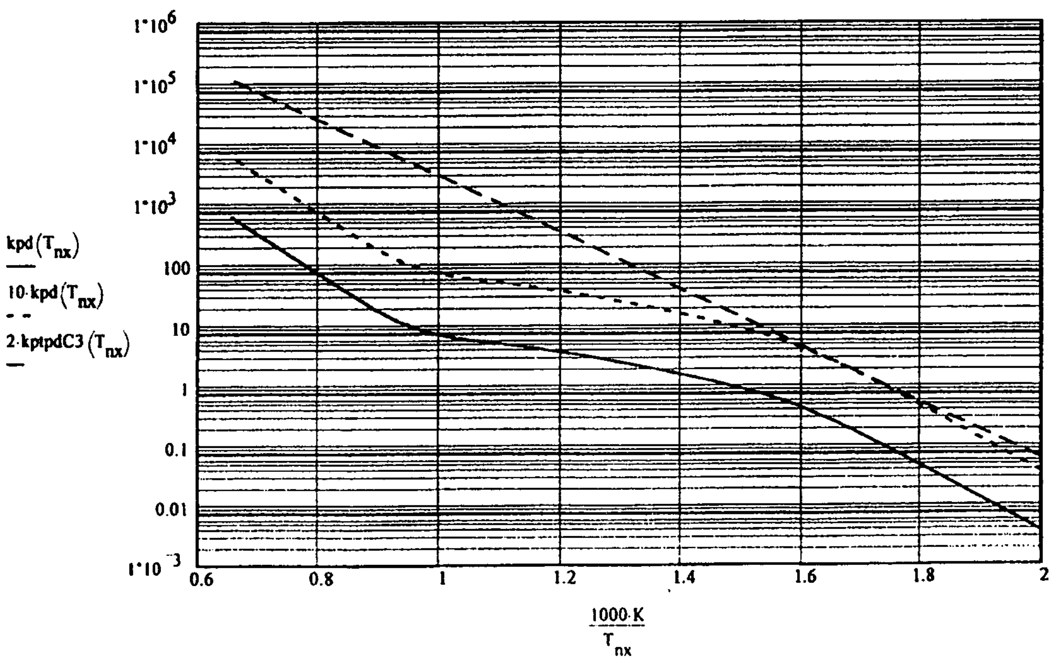
$$kptpdC3(T) := 6.9 \cdot 10^{4} \cdot \exp\left(-\frac{10760 \cdot K}{T}\right) \cdot gm^{-1} \cdot sec^{-1}$$

$10 \cdot kpd(900 \cdot K) = 49.2392 \cdot kg^{-1} \cdot sec^{-1}$

$2 \cdot kptpdC3(900 \cdot K) = 886.4358 \cdot kg^{-1} \cdot sec^{-1}$

$nx := 0, 1 .. 41 \qquad T_{nx} := 500 \cdot K + nx \cdot 25 \cdot K$

CATALYTIC RATE CONSTANT vs TEMPERATURE (mol/atmCHx/s/gcat)



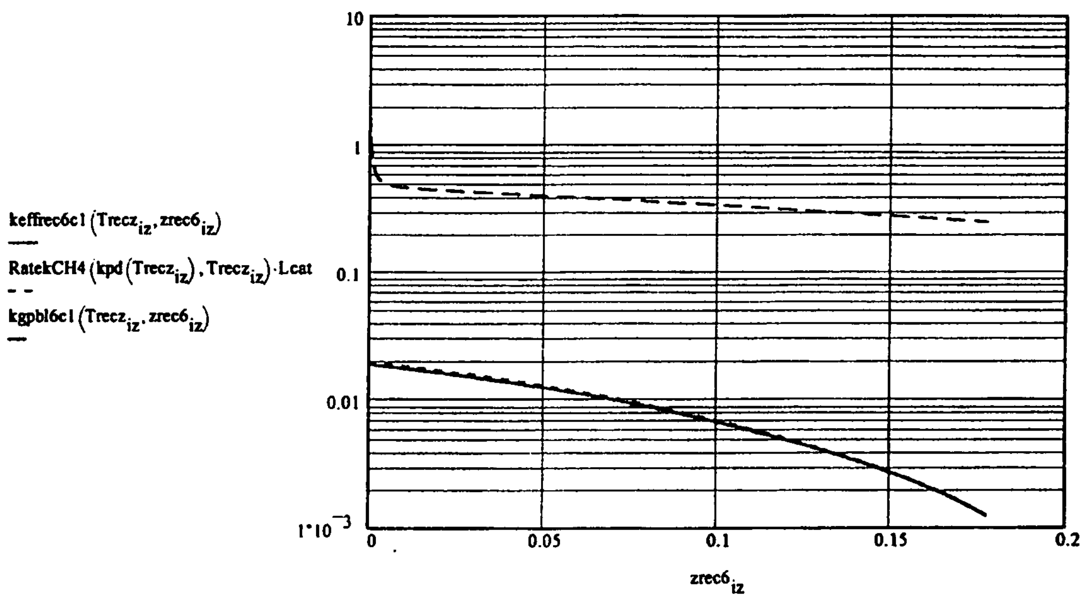
B4

$$\mathrm{keffrec6c1}(T,z) := \frac{1}{\left(\frac{1}{\mathrm{RatekCH4}(\mathrm{kpd}(T),T)\cdot \mathrm{Lcat}}\right)+\frac{1}{\mathrm{kgpbl6c1}(T,z)}} \qquad \mathrm{kgpbl6c1}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 35.3023\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$$

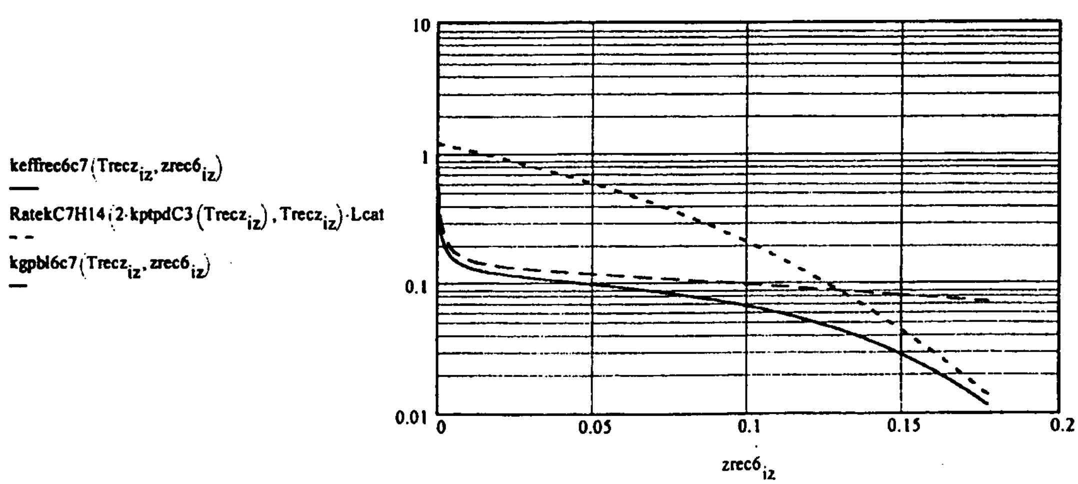
$$\mathrm{keffrec6c1}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 0.7922\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm} \qquad \mathrm{RatekCH4}\left(\mathrm{kpd}\left(\mathrm{Tavg}_{\mathrm{ncase}}\right),\mathrm{Tavg}_{\mathrm{ncase}}\right)\cdot \mathrm{Lcat} = 0.8104\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$$

$$\mathrm{keffrec6c7}(T,z) := \frac{1}{\left(\frac{1}{\mathrm{RatekC7H14}(2\cdot \mathrm{kptpdC3}(T),T)\cdot \mathrm{Lcat}}\right)+\frac{1}{\mathrm{kgpbl6c7}(T,z)}} \qquad \mathrm{kgpbl6c7}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 10.1756\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm}$$

$$\mathrm{keffrec6c7}\left(\mathrm{Tavg}_{\mathrm{ncase}},\frac{\mathrm{Lrec}}{2}\right) = 7.4067\cdot \mathrm{sec}^{-1}\cdot \mathrm{cm} \qquad \mathrm{RatekC7H14}\left(2\cdot \mathrm{kptpdC3}\left(\mathrm{Tavg}_{\mathrm{ncase}}\right),\mathrm{Tavg}_{\mathrm{ncase}}\right)\cdot \mathrm{Lcat} = 27.2196\cdot \mathrm{sec}^{-1}$$



Case specific ncase = 5



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $ncase = 5$

$$Trecz_{iz} := Trecin_{ncase} - \frac{Trecin_{ncase} - Trecout_{ncase}}{nz} \cdot iz \qquad Trecz_{nz} = 630.3722 \cdot K \qquad Trecout_{ncase} = 630.3722 \cdot K$$

$$yzkc7h14_0 := yc7h140 \qquad yzkch4_0 := ych40$$

$$yzkc7h14_{iz+1} := \left(1 - keffrec6c7\left(Trecz_{iz}, zrec6_{iz}\right) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}}\right) \cdot yzkc7h14_{iz}$$

Case specific

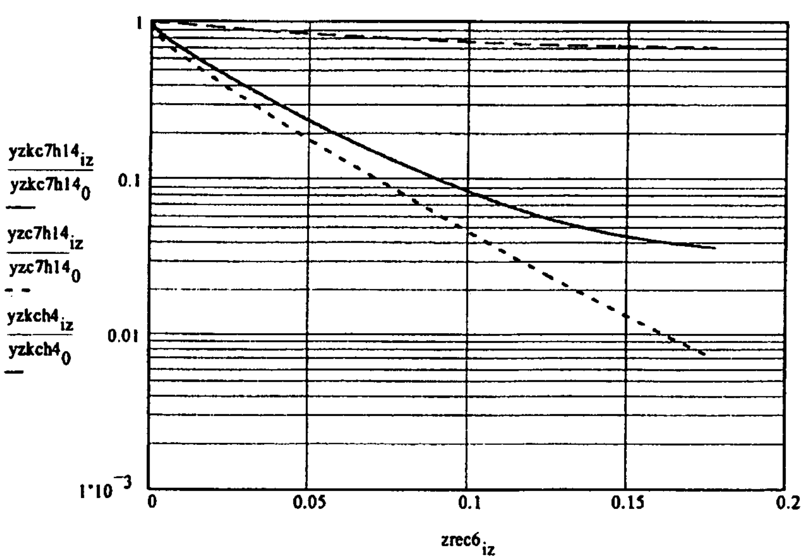
$ncase = 5$

$$yzkch4_{iz+1} := \left(1 - keffrec6c1\left(Trecz_{iz}, zrec6_{iz}\right) \cdot \frac{Lrec}{nz} \cdot 1.1 \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell6}{Urec_{ncase}} \cdot \frac{Trecin_5}{Trecz_{iz}}\right) \cdot yzkch4_{iz}$$

Case specific

$$yzkc7h14_{nz} = 1.802 \cdot 10^{-5} \qquad yzkc7h14_0 = 0.0005 \qquad \frac{yzkc7h14_{nz}}{yzkc7h14_0} = 3.603 \cdot 10^{-2} \qquad \frac{yzkch4_{nz}}{yzkch4_0} = 0.6838$$

$$yzkch4_{nz} = 0.0034 \qquad yzkch4_0 = 0.005$$



Case specific $ncase = 5$

Conversion of C7H14 under case 5 (full power) is 97.4% with estimated catalytic rates and transport limitations [vs. 99.6% for the maximum BL transport-limited conversion]. Conversion of CH4 is very poor (32%). CO conversion is probably very high given higher catalytic and transport rates than with C7H14.

This result shows that the specific rates of catalytic oxidation of all added components needs to be measured as applied to a recuperator. The use of a recuperator for emission control would appear to be greatly enhanced with higher exhaust (recuperator) temperatures.

In the following section, the conversion of C7H14, CH4 and CO is considered for various honeycomb monliths

$$Thc_{jcase+1} := Trecin_{jcase+1} \qquad \rho mixhc_{jcase+1} := \rho mixrec\left(Trecin_{jcase+1}\right)$$

$$Ghc2_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell2} \qquad Ghc4_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell4} \qquad Ghc6_{jcase+1} := \frac{mf_{jcase+1}}{Shc \cdot \varepsilon cell6}$$

$$Uhc2 = \begin{bmatrix} 0 \\ 3.058 \\ 3.9753 \\ 4.801 \\ 5.8101 \\ 10.0353 \end{bmatrix} \cdot m \cdot sec^{-1} \qquad Uhc4 = \begin{bmatrix} 0 \\ 3.2157 \\ 4.1804 \\ 5.0487 \\ 6.1098 \\ 10.553 \end{bmatrix} \cdot m \cdot sec^{-1} \qquad Uhc6 = \begin{bmatrix} 0 \\ 3.1706 \\ 4.1218 \\ 4.9779 \\ 6.0242 \\ 10.4051 \end{bmatrix} \cdot m \cdot sec^{-1}$$

Evaluate Reynolds numbers for use in calculating the momentum, heat, and mass transfer functions:

$$Rehc2_{jcase+1} := \frac{Ghc2_{jcase+1} \cdot dcell2}{\mu mixT\left(Thc_{jcase+1}\right)} \qquad Rehc4_{jcase+1} := \frac{Ghc4_{jcase+1} \cdot dcell4}{\mu mixT\left(Thc_{jcase+1}\right)} \qquad Rehc6_{jcase+1} := \frac{Ghc6_{jcase+1} \cdot dcell6}{\mu mixT\left(Thc_{jcase+1}\right)}$$

$$Rehc2 = \begin{bmatrix} 0 \\ 43.776 \\ 56.9088 \\ 68.7283 \\ 83.1744 \\ 167.4548 \end{bmatrix} \qquad Rehc4 = \begin{bmatrix} 0 \\ 31.7427 \\ 41.2655 \\ 49.836 \\ 60.3111 \\ 121.4242 \end{bmatrix} \qquad Rehc6 = \begin{bmatrix} 0 \\ 25.7355 \\ 33.4562 \\ 40.4048 \\ 48.8975 \\ 98.4453 \end{bmatrix}$$

$$cfrichc2(j,z) := \frac{14.227}{Rehc2_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc2_j \cdot \frac{dcell2}{z}\right)\right]^{0.45363}$$

$$cfrichc4(j,z) := \frac{14.227}{Rehc4_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc4_j \cdot \frac{dcell4}{z}\right)\right]^{0.45363}$$

Average coefficients of friction for smooth square channels

$$cfrichc6(j,z) := \frac{14.227}{Rehc6_j} \cdot \left[1 + 0.046263 \cdot \left(Rehc6_j \cdot \frac{dcell6}{z}\right)\right]^{0.45363}$$

Calculate monolith pressure drop in recuperator with entrance effect:

$$\Delta Phc2_{jcase+1} := 4 \cdot cfrichc2(jcase+1, Lhc) \cdot \frac{\left(Uhc2_{jcase+1}\right)^2}{2} \cdot \rho mixhc_{jcase+1} \cdot \frac{Lhc}{dcell2}$$

$$\Delta Phc4_{jcase+1} := 4 \cdot cfrichc4(jcase+1, Lhc) \cdot \frac{\left(Uhc4_{jcase+1}\right)^2}{2} \cdot \rho mixhc_{jcase+1} \cdot \frac{Lhc}{dcell4}$$

$$\Delta Phc6_{jcase+1} := 4 \cdot cfrichc6(jcase+1, Lhc) \cdot \frac{\left(Uhc6_{jcase+1}\right)^2}{2} \cdot \rho mixhc_{jcase+1} \cdot \frac{Lhc}{dcell6}$$

$$\frac{\Delta Phc2}{Phc} = \begin{bmatrix} 0 \\ 0.0013 \\ 0.0017 \\ 0.002 \\ 0.0024 \\ 0.0041 \end{bmatrix} \quad \frac{\Delta Phc4}{Phc} = \begin{bmatrix} 0 \\ 0.0028 \\ 0.0036 \\ 0.0044 \\ 0.0053 \\ 0.0088 \end{bmatrix} \quad \frac{\Delta Phc6}{Phc} = \begin{bmatrix} 0 \\ 0.004 \\ 0.0053 \\ 0.0064 \\ 0.0077 \\ 0.0127 \end{bmatrix} \quad \frac{3.5}{4} \cdot \frac{\Delta Phc6}{Phc} = \begin{bmatrix} 0 \\ 0.0035 \\ 0.0046 \\ 0.0056 \\ 0.0068 \\ 0.0111 \end{bmatrix} \quad \Delta Phcmax\_P := \begin{bmatrix} 0 \\ 0.003 \\ 0.004 \\ 0.005 \\ 0.006 \\ 0.011 \end{bmatrix}$$

Chose 600 cells per in2 honeycombs but reduce length to 3.5in via estimated ΔP $Lhc := 3.5 \cdot in$

****

Use 600 cells/in2 in honeycomb monolith for calculation of CH4, C7H14, and CO conversions

Find mass transfer rates via Nusselt formulas:

$$Numavghc6c1_{jcase+1} := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc6_{jcase+1} \cdot Sc1T\left(Thc_{jcase+1}\right) \cdot dcell6}\right)^{-\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavghc6c1 = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9767 \end{bmatrix}$$

$$Numavghc6co_{jcase+1} := 2.976 \cdot \left[1 + \left(\frac{7.6 \cdot Lhc}{Rehc6_{jcase+1} \cdot SccoT\left(Thc_{jcase+1}\right) \cdot dcell6}\right)^{-\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavghc6co = \begin{bmatrix} 0 \\ 2.976 \\ 2.976 \\ 2.9761 \\ 2.9761 \\ 2.9769 \end{bmatrix}$$

****

$$Numavghc6c7_{jcase+1} := 2.976\cdot\left[1+\left(\frac{7.6\cdot Lhc}{Rehc6_{jcase+1}\cdot Sc7T\left(Thc_{jcase+1}\right)\cdot dcell6}\right)^{\frac{8}{3}}\right]^{\frac{1}{8}} \qquad Numavghc6c7 = \begin{pmatrix} 0 \\ 2.9765 \\ 2.977 \\ 2.9777 \\ 2.9788 \\ 2.994 \end{pmatrix}$$

Once again the entrance effects within monoliths are generally small

Now determine the maximum possible CH4, C7H14, and CO conversions in a 600 cells per in2 monolith

$ych40 := 0.005 \qquad yc7h140 := 0.0005 \qquad yco0 := 0.005$

$$ych4hc6_{jcase+1} := ych40\cdot\exp\left(\frac{-4\cdot Lhc\cdot Numavghc6c1_{jcase+1}}{Rehc6_{jcase+1}\cdot Sc1T\left(Thc_{jcase+1}\right)\cdot dcell6}\right)$$

$$\frac{-4\cdot Lhc\cdot Numavghc6c1_{jcase+1}}{Rehc6_{jcase+1}\cdot Sc1T\left(Thc_{jcase+1}\right)\cdot dcell6}$$

-64.0074
-49.2367
-40.7696
-33.689
-16.7076

$$\frac{ych4hc6}{ych40} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 2.339\cdot 10^{-15} \\ 5.5463\cdot 10^{-8} \end{pmatrix}$$

$$ycohc6_{jcase+1} := yco0\cdot\exp\left(\frac{-4\cdot Lhc\cdot Numavghc6co_{jcase+1}}{Rehc6_{jcase+1}\cdot SccoT\left(Thc_{jcase+1}\right)\cdot dcell6}\right)$$

$$\frac{ycohc6}{yco0} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 4.7906\cdot 10^{-14} \\ 2.445\cdot 10^{-7} \end{pmatrix}$$

$$\frac{-4\cdot Lhc\cdot Numavghc6co_{jcase+1}}{Rehc6_{jcase+1}\cdot SccoT\left(Thc_{jcase+1}\right)\cdot dcell6}$$

-58.27
-44.8234
-37.1153
-30.6695
-15.2241

$$yc7h14hc6_{jcase+1} = yc7h140 \cdot \exp\left(\frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell6}\right)$$

$$\frac{-3.5 \cdot Lhc \cdot Numavghc6c7_{jcase+1}}{Rehc6_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell6} = \begin{array}{|c|}\hline -16.2974 \\ \hline -12.5386 \\ \hline -10.3846 \\ \hline -8.5841 \\ \hline -4.2631 \\ \hline \end{array}$$

$$\frac{yc7h14hc6}{yc7h140} = \begin{bmatrix} 0 \\ 8.3588 \cdot 10^{-8} \\ 3.5856 \cdot 10^{-6} \\ 3.0905 \cdot 10^{-5} \\ 0.0002 \\ 0.0141 \end{bmatrix}$$

Only for C7H14 and only in case 5 (maximum power) does the BL transport-only calculated conversion (98.6%) fall below 99.9% with a 600 cells/in2 monolith With 50 ppm C7H14 in the exhaust in this case, the exit concentration would be 0.7 ppm.

****

For the final analysis, consider the finite catalytic conversion of C7H14 and CH4 in a monolith: $mcase := 5$

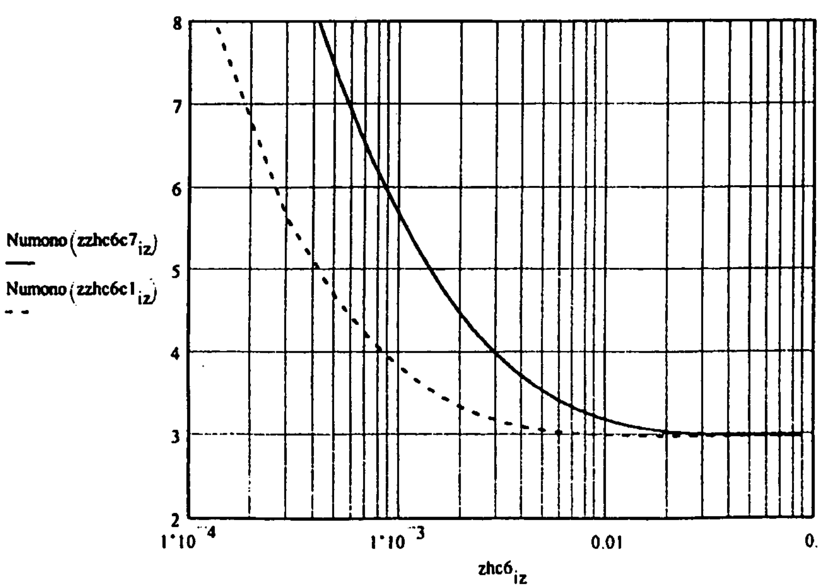
$$zzcharhc6c7_{jcase+1} := \frac{Rehc6_{jcase+1} \cdot Sc7T\left(Thc_{jcase+1}\right) \cdot dcell6}{2} \qquad \frac{Lhc}{zzcharhc6c7_{mcase}} = 0.8137$$

$$zzcharhc6c1_{jcase+1} := \frac{Rehc6_{jcase+1} \cdot Sc1T\left(Trecin_{jcase+1}\right) \cdot dcell6}{2} \qquad \frac{Lhc}{zzcharhc6c1_{mcase}} = 2.8064$$

$nz = 400$ $\quad Lhc = 8.89 \cdot cm$ $\quad dcell6 = 0.0961 \cdot cm$

$$zhc6_{iz} := iz \cdot \frac{Lhc}{nz} + dwall6 \qquad zzhc6c7_{iz} := \frac{zhc6_{iz}}{zzcharhc6c7_{mcase}} \qquad zzhc6c1_{iz} := \frac{zhc6_{iz}}{zzcharhc6c1_{mcase}}$$

$$zzcharhc6c7 = \begin{bmatrix} 0 \\ 2.8414 \\ 3.6938 \\ 4.461 \\ 5.3986 \\ 10.926 \end{bmatrix} \cdot cm$$



Case specific $mcase = 5$

$$kgpblhc6c7(T,z) := \frac{Dc7h14T(T)\cdot Numono\left(\frac{z}{zzcharhc6c7_{mcase}}\right)}{dcell6}$$

$$kgpblhc6c7\left(Thc_{mcase}, Lhc\right) = 13.6172\cdot sec^{-1}\cdot cm$$

$$kgpblhc6c1(T,z) := \frac{Dch4T(T)\cdot Numono\left(\frac{z}{zzcharhc6c1_{mcase}}\right)}{dcell6}$$

$$kgpblhc6c1\left(Thc_{mcase}, Lhc\right) = 46.9581\cdot sec^{-1}\cdot cm$$

$$keffhc6c1(T,z) := \frac{1}{\left(\frac{1}{RatekCH4(kpd(T),T)\cdot Lcat}\right) + \frac{1}{kgpblhc6c1(T,z)}}$$

$$kgpblhc6c1\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 46.9589\cdot sec^{-1}\cdot cm$$

$$keffhc6c1\left(Thc_{mcase}, \frac{Lrec}{2}\right) = 1.8693\cdot sec^{-1}\cdot cm$$

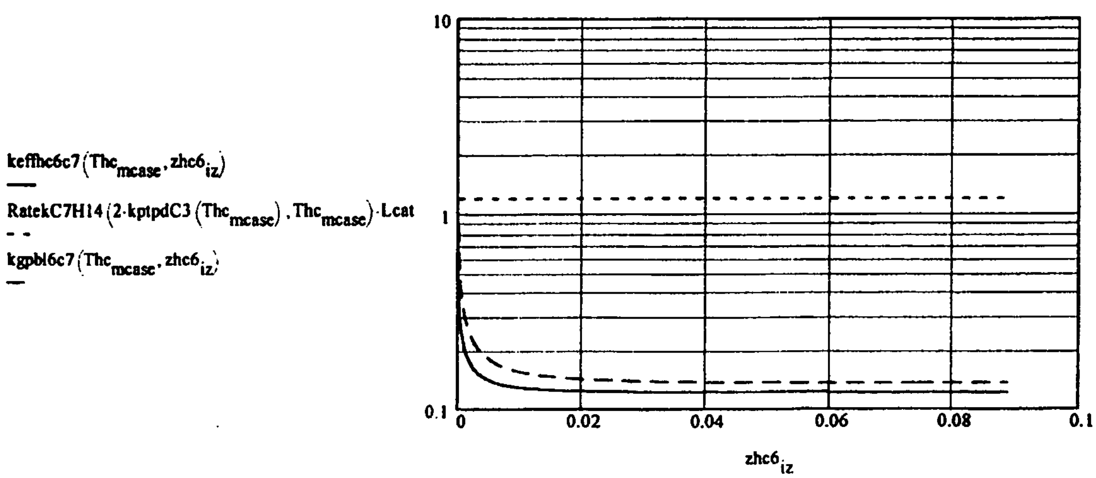
$$RatekCH4\left(kpd\left(Thc_{mcase}\right), Thc_{mcase}\right)\cdot Lcat = 1.9467\cdot sec^{-1}\cdot cm$$

$$keffhc6c7(T,z) := \frac{1}{\left(\frac{1}{RatekC7H14(2\cdot kptpdC3(T),T)\cdot Lcat}\right) + \frac{1}{kgpblhc6c7(T,z)}}$$

$$kgpblhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 13.6468\cdot sec^{-1}\cdot cm$$

$$keffhc6c7\left(Thc_{mcase}, \frac{Lhc}{2}\right) = 12.2537\cdot sec^{-1}\cdot cm$$

$$RatekC7H14\left(2\cdot kptpdC3\left(Thc_{mcase}\right), Thc_{mcase}\right)\cdot Lcat = 120.0371\cdot sec^{-1}\cdot cm$$



Determine conversion of fuels with transport-limited finite catalytic combustion rates:

Case specific $mcase = 5$

$yzkhc6c7h14_0 := yc7h140$ $yzkhc6ch4_0 := ych40$

$$Thc = \begin{pmatrix} 0 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 1005.3722 \\ 916.4833 \end{pmatrix} \cdot K$$

$$yzkhc6c7h14_{iz+1} := \left(1 - keffhc6c7\left(Thc_{mcase}, zhc6_{iz}\right) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell6}{Uhc6_{mcase}}\right) \cdot yzkhc6c7h14_{iz}$$

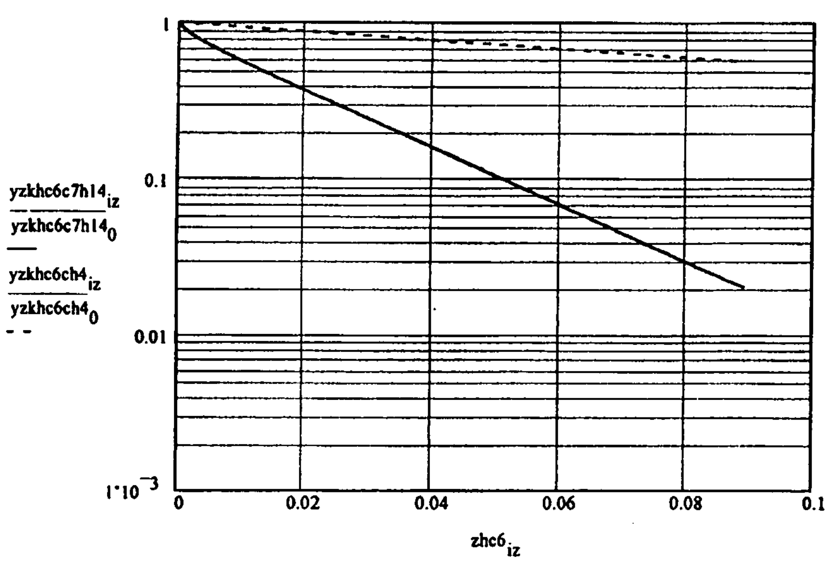
$$yzkhc6ch4_{iz+1} := \left(1 - keffhc6c1\left(Thc_{mcase}, zhc6_{iz}\right) \cdot \frac{Lhc}{nz} \cdot \frac{4}{dcell6} \cdot \frac{\varepsilon cell4}{Uhc6_{mcase}}\right) \cdot yzkhc6ch4_{iz}$$

Case specific

$mcase = 5$

$yzkhc6c7h14_{nz} = 9.964 \cdot 10^{-6}$ $yzkhc6c7h14_0 = 0.0005$

$yzkhc6ch4_{nz} = 0.0028$ $yzkhc6ch4_0 = 0.005$ $\frac{yzkhc6c7h14_{nz}}{yzkhc6c7h14_0} = 1.993 \cdot 10^{-2}$ $\frac{yzkhc6ch4_{nz}}{yzkhc6ch4_0} = 0.5693$



Case specific $mcase = 5$

Conversion of C7H14 under case 5 (full power) with 600 cells/in2 x 3.5-in length and extrapolated catalytic rates (via C3H8 at 400C) is 98.0% (vs. 99.6% via averaged integrated formulas, 99.3% with temperature dependent transport, and 98.6% with 400 cells/in2 and 4-in length. Conversion of CH4 is limited by slow kinetics and CO is expected to be very high (>99.99%).

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Gas Properties and Constants

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$cm \equiv 0.01 \cdot m$ $J \equiv kg \cdot m^2 \cdot sec^{-2}$ $W \equiv J \cdot sec^{-1}$ $Pref := 1 \cdot atm$

$N \equiv kg \cdot m \cdot sec^{-2}$ $Pa \equiv N \cdot m^{-2}$ $atm \equiv 101300 \cdot Pa$ $\mu m \equiv 0.000001 \cdot m$

$R := 8.3143 \cdot \frac{J}{K}$ $Rc := 8.3143 \cdot J \cdot mole^{-1} \cdot K^{-1}$

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n	Gas	MolWt	σ(LJ)	ε(LJ)
1	CH4	$MW_0 := 16.044 \cdot gm$	$\sigma_0 := 3.785 \cdot 10^{-10} \cdot m$	$\varepsilon_0 := 148.6 \cdot K$
2	O2	$MW_1 := 31.999 \cdot gm$	$\sigma_1 := 3.464 \cdot 10^{-10} \cdot m$	$\varepsilon_1 := 106.7 \cdot K$
3	N2	$MW_2 := 28.018 \cdot gm$	$\sigma_2 := 3.798 \cdot 10^{-10} \cdot m$	$\varepsilon_2 := 71.4 \cdot K$
4	CO2	$MW_3 := 44.010 \cdot gm$	$\sigma_3 := 3.941 \cdot 10^{-10} \cdot m$	$\varepsilon_3 := 195.2 \cdot K$
5	H2O	$MW_4 := 18.015 \cdot gm$	$\sigma_4 := 2.641 \cdot 10^{-10} \cdot m$	$\varepsilon_4 := 809.1 \cdot K$

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Define transport integrals:

Constants:

$\sigma\mu a_0 := 1.16145$ $\sigma\mu b_0 := 0.14874$ $\sigma Da_0 := 1.06036$ $\sigma Db_0 := 0.1561$

$\sigma\mu a_1 := 0.52487$ $\sigma\mu b_1 := 0.7732$ $\sigma Da_1 := 0.193$ $\sigma Db_1 := 0.47635$

$\sigma\mu a_2 := 2.16178$ $\sigma\mu b_2 := 2.43787$ $\sigma Da_2 := 1.03587$ $\sigma Db_2 := 1.52996$

$\sigma Da_3 := 1.76474$ $\sigma Db_3 := 3.89411$

Functions:

$$\Omega\mu(T) := \sigma\mu a_0 \cdot \exp\left[-\left(\sigma\mu b_0 \cdot \ln(T)\right)\right] + \sum_{i\mu=1}^{2} \sigma\mu a_{i\mu} \cdot \exp\left(-\sigma\mu b_{i\mu} \cdot T\right) \qquad \Omega\mu(3) = 1.0394$$

$$\Omega D(T) := \sigma Da_0 \cdot \exp\left[-\left(\sigma Db_0 \cdot \ln(T)\right)\right] + \sum_{iD=1}^{3} \sigma Da_{iD} \cdot \exp\left(-\sigma Db_{iD} \cdot T\right) \qquad \Omega D(3) = 0.95002$$

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B5
~~B4~~

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Set Inlet Conditions:

$P := 1.0 \cdot atm \qquad ych40 := 0.035$

Define gas composition w/r methane using moist (3%) air:

$$y(x) := \begin{bmatrix} x \\ (1 - ych40) \cdot 0.2 - 2 \cdot ych40 + 2 \cdot x \\ (1 - ych40) \cdot 0.77 \\ ych40 - x \\ (1 - ych40) \cdot 0.03 + 2 \cdot ych40 - 2 \cdot x \end{bmatrix} \qquad y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

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Define viscosity function

$$\mu(T) := \begin{bmatrix} 2.6693 \cdot 10^{-26} \cdot \dfrac{(MW_0 \cdot T)^{0.5}}{(\sigma_0)^2 \cdot \Omega\mu\left(\dfrac{T}{\varepsilon_0}\right)} \cdot \dfrac{10^5 \cdot cm}{sec} \cdot \left(\dfrac{gm}{K}\right)^{0.5} \\ \dfrac{(MW_1 \cdot T)^{0.5}}{(\sigma_1)^2 \cdot \Omega\mu\left(\dfrac{T}{\varepsilon_1}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\dfrac{10^5 \cdot cm}{sec}\right) \cdot \left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{(MW_2 \cdot T)^{0.5}}{(\sigma_2)^2 \cdot \Omega\mu\left(\dfrac{T}{\varepsilon_2}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\dfrac{10^5 \cdot cm}{sec}\right) \cdot \left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{(MW_3 \cdot T)^{0.5}}{(\sigma_3)^2 \cdot \Omega\mu\left(\dfrac{T}{\varepsilon_3}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\dfrac{10^5 \cdot cm}{sec}\right) \cdot \left(\dfrac{gm}{K}\right)^{0.5}\right] \\ \dfrac{1.116 \cdot (MW_4 \cdot T)^{0.5}}{(3.115 \cdot 10^{-8} \cdot cm)^2 \cdot \Omega\mu\left(\dfrac{T}{514 \cdot K}\right)} \cdot \left[2.6693 \cdot 10^{-26} \cdot \left(\dfrac{10^5 \cdot cm}{sec}\right) \cdot \left(\dfrac{gm}{K}\right)^{0.5}\right] \end{bmatrix} \qquad \mu(300 \cdot K) = \begin{bmatrix} 1.103 \cdot 10^{-5} \\ 2.06 \cdot 10^{-5} \\ 1.77 \cdot 10^{-5} \\ 1.519 \cdot 10^{-5} \\ 1.068 \cdot 10^{-5} \end{bmatrix} \cdot kg \cdot m^{-1} \cdot sec^{-1}$$

$$\mu mix(x,T) := \sum_{n=0}^{4} \frac{y(x)_n \cdot (\mu(T))_n}{\displaystyle\sum_{m=0}^{4} y(x)_m \cdot \left[\frac{\left[1 + \left(\frac{\mu(T)_n}{\mu(T)_m}\right)^{0.5} \cdot \left(\frac{MW_m}{MW_n}\right)^{0.25}\right]^2}{\left[8\cdot\left(1+\frac{MW_n}{MW_m}\right)\right]^{0.5}} \right]}$$

$$y(0.02) = \begin{bmatrix} 0.02 \\ 0.163 \\ 0.743 \\ 0.015 \\ 0.059 \end{bmatrix}$$

$$\mu mix(0.02, 300\cdot K) = 1.759\cdot 10^{-5}\cdot kg\cdot m^{-1}\cdot sec^{-1}$$

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Define thermal conductivity functions

$igas := 0, 1 .. 4$

$$a\lambda := \begin{bmatrix} -1.869 \\ -.3273 \\ 0.3919 \\ -7.215 \\ 7.341 \end{bmatrix} \quad b\lambda := \begin{bmatrix} 0.08727 \\ 0.09966 \\ 0.09816 \\ 0.08015 \\ -0.01013 \end{bmatrix} \quad c\lambda := \begin{bmatrix} 1.179\cdot 10^{-4} \\ -\left(3.743\cdot 10^{-5}\right) \\ -\left(5.067\cdot 10^{-5}\right) \\ 5.477\cdot 10^{-6} \\ 1.801\cdot 10^{-4} \end{bmatrix} \quad d\lambda := \begin{bmatrix} -\left(3.614\cdot 10^{-8}\right) \\ 9.732\cdot 10^{-9} \\ 1.504\cdot 10^{-8} \\ -\left(1.053\cdot 10^{-8}\right) \\ -\left(9.1\cdot 10^{-8}\right) \end{bmatrix} \begin{array}{l} CH4 \\ O2 \\ N2 \\ CO2 \\ H2O \end{array}$$

$$\lambda(i,T) := \left[a\lambda_i + b\lambda_i\cdot\frac{T}{K} + c\lambda_i\cdot\left(\frac{T}{K}\right)^2 + d\lambda_i\cdot\left(\frac{T}{K}\right)^3\right]\cdot 0.00001\cdot\frac{W}{cm\cdot K}$$ W/cm/K

$\lambda(igas, 1000\cdot K)$

$0.16716\cdot kg\cdot m\cdot sec^{-3}\cdot K^{-1}$
$0.07163\cdot kg\cdot m\cdot sec^{-3}\cdot K^{-1}$
$0.06292\cdot kg\cdot m\cdot sec^{-3}\cdot K^{-1}$
$0.06788\cdot kg\cdot m\cdot sec^{-3}\cdot K^{-1}$
$0.08631\cdot kg\cdot m\cdot sec^{-3}\cdot K^{-1}$

$$\lambda mix(x,T) := \sum_{i=0}^{4} \frac{y(x)_i \cdot \lambda(i,T)}{\displaystyle\sum_{j=0}^{4} y(x)_j \cdot \left[\frac{\left[1 + \left(\frac{\mu(T)_i}{\mu(T)_j}\right)^{0.5} \cdot \left(\frac{MW_j}{MW_i}\right)^{0.25}\right]^2}{\left[8\cdot\left(1+\frac{MW_i}{MW_j}\right)\right]^{0.5}} \right]}$$

$$\lambda mix(.0, 1000\cdot K) = 6.64\cdot 10^{-4}\cdot\frac{W}{cm\cdot K}$$

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Define thermal conductivity of alumina and SS321

$$\text{Altc} := \begin{bmatrix} 83.71 \\ -224.898 \\ 255.842 \\ -132.727 \\ 25.9695 \end{bmatrix}$$

The parameter set Altc_n was determined from published values of the thermal conductivity. Ref: HCP

λAl2O3(x) is the thermal conductivity function (of x with unit K) while λ1 is its derivative w/r to temperature.

$$\lambda Al2O3(x) := \sum_{n=0}^{4} \text{Altc}_n \cdot \left(\frac{x}{1000 \cdot K}\right)^n \cdot \frac{W}{m \cdot K} \qquad \lambda 1(x) := \sum_{n=1}^{4} \frac{\text{Altc}_n}{1000 \cdot K} \cdot n \cdot \left(\frac{x}{1000 \cdot K}\right)^{n-1} \cdot \frac{W}{m \cdot K}$$

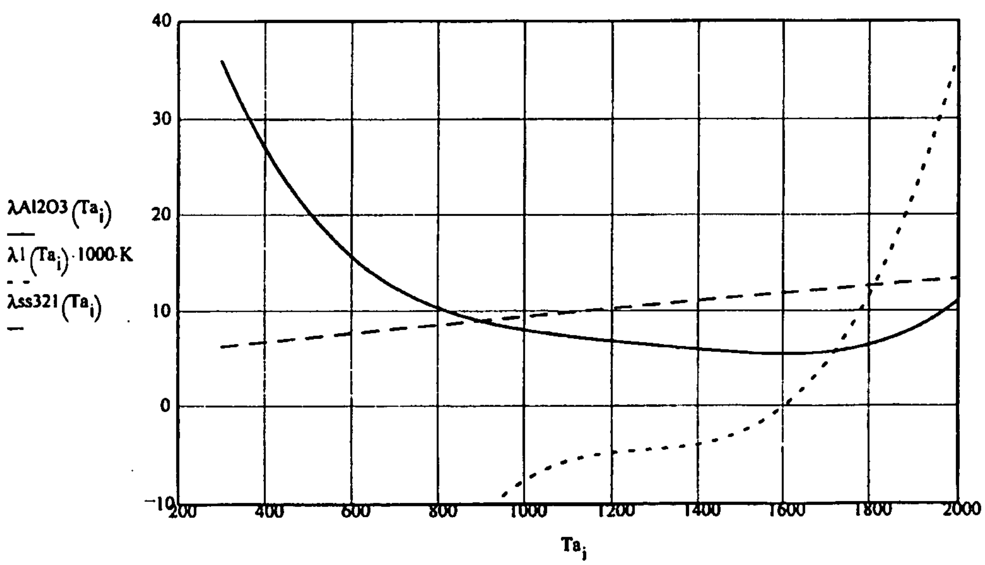
$$\text{S321tc} := \begin{bmatrix} 4.69312 \\ 4.9812 \\ -0.33357 \\ 0 \\ 0 \end{bmatrix}$$

The parameter set S321tc_n was determined from published values of the thermal conductivity. Ref: Handbook of Metals 8th Ed. Vol. 1 p. 423

$$\lambda ss321(x) := \sum_{n=0}^{4} \text{S321tc}_n \cdot \left(\frac{x}{1000 \cdot K}\right)^n \cdot \frac{W}{m \cdot K}$$

$$\lambda ss321(1000 \cdot K) = 9.341 \cdot \frac{W}{m \cdot K} \qquad \lambda Al2O3(1000 \cdot K) = 7.897 \cdot \frac{W}{m \cdot K} \qquad \lambda 1(1000 \cdot K) \cdot 1000 \cdot K = -7.517 \cdot \frac{W}{m \cdot K}$$

$i := 30, 31 .. 200$ $\qquad$ $Ta_i := 10 \cdot i \cdot K$



$x := 1500 \cdot K \qquad x0 \quad root(\lambda 1(x), x) \qquad x0 = 1.588 \cdot 10^{3} K$

$\lambda ss321(300 \cdot K) = 6.157 \cdot \frac{W}{m \cdot K} \qquad 0.003 \cdot in = 7.62 \cdot 10^{-3} \cdot cm$

$\lambda Al2O3(300 \cdot K) = 0.359 \cdot \frac{W}{cm \cdot K} \qquad \lambda Al2O3(200 \cdot K) = 0.479 \cdot \frac{W}{cm \cdot K}$

$\lambda Al2O3(800 \cdot K) = 0.102 \cdot \frac{W}{cm \cdot K} \qquad \lambda Al2O3(x0) = 0.054 \cdot \frac{W}{cm \cdot K}$ Minimum thermal conductivity

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Determine thermal conductivity of porous wall:

Ref: RHG - Handbook Chpt 6 for effective thermal conductivity including convection and radiative terms

$\varepsilon rad := 0.6 \qquad \varepsilon := 0.42 \qquad dp := 0.00005 \cdot cm \qquad dp = 5 \cdot 10^{-7} \cdot m$

$$\lambda wc(x,T) := \lambda mix(x,T) \cdot \left[0.0931 + 2 \cdot 0.9069 \cdot \left(\frac{\lambda Al2O3(T)}{\lambda Al2O3(T) - \lambda mix(x,T)} \right)^2 \cdot \left(\ln\left(\frac{\lambda Al2O3(T)}{\lambda mix(x,T)} \right) - 1 \right) \right] \ldots$$
$$+ 0.229 \cdot 10^{-6} \cdot \frac{W}{m^2 \cdot K^4} \cdot \varepsilon \cdot dp \cdot \varepsilon rad \cdot T^3 \cdot \left[\varepsilon + \frac{1 - \varepsilon}{\left(\frac{0.229 \cdot 10^{-6} \cdot \frac{W}{m^2 \cdot K^4} \cdot \varepsilon \cdot dp \cdot \varepsilon rad \cdot T^3}{\lambda Al2O3(T)} + 1 \right)} \right]$$

$$\lambda wcnr(x,T) := \lambda mix(x,T) \cdot \left[0.0931 + 2 \cdot 0.9069 \cdot \left(\frac{\lambda Al2O3(T)}{\lambda Al2O3(T) - \lambda mix(x,T)} \right)^2 \cdot \left(\ln\left(\frac{\lambda Al2O3(T)}{\lambda mix(x,T)} \right) - 1 \right) \right]$$

$\lambda wc(0.01, 1000 \cdot K) = 0.473 \cdot \frac{W}{m \cdot K} \qquad \lambda wcnr(0.01, 1000 \cdot K) = 0.473 \cdot \frac{W}{m \cdot K}$ Radiation component negligible with such small particles in the washcoat

$\lambda mix(0.01, 1000 \cdot K) = 0.067 \cdot \frac{W}{m \cdot K} \qquad \lambda Al2O3(700 \cdot K) = 12.354 \cdot \frac{W}{m \cdot K} \qquad \lambda ss321(1000 \cdot K) = 9.341 \cdot \frac{W}{m \cdot K}$

$$\frac{\lambda Al2O3(1000\cdot K)}{\lambda mix(0.01,1000\cdot K)}=117.74 \qquad \frac{\lambda wc(0.01,1000\cdot K)}{\lambda mix(0.01,1000\cdot K)}=7.046$$

The thermal conductivity of the wash coat is about 7 times greater at 1000K than the gas phase conductivity

$$\frac{\lambda wc(0.01,1000\cdot K)}{\lambda ss321(1000\cdot K)}=0.051 \qquad \frac{\dfrac{\lambda wc(0.01,1000\cdot K)}{0.001\cdot cm}+\dfrac{\lambda ss321(1000\cdot K)}{0.003\cdot in}}{\dfrac{\lambda ss321(1000\cdot K)}{0.003\cdot in}}=1.386$$

The washcoat increases the thermal conductance of the wall by about 39%

$$\frac{\lambda ss321(1000\cdot K)}{\lambda mix(0.01,1000\cdot K)}=139.275$$

For a Nusselt no. of 2.976 (dcell8 = 0.0961*cm) for developed flow in the recuperator (full power) the mean heat transfer boundary layer thickness is much greater than either the SS321 wall thickness or the washcoat thickness.

$$\delta gprecup := \frac{0.0961\cdot cm}{2.976} \qquad \delta gprecup = 0.032\cdot cm$$

$$hrecavg(T) := \frac{1}{\left(\dfrac{2}{\dfrac{\lambda mix(0.01,T)}{\delta gprecup}}\right)+\dfrac{1}{\dfrac{\lambda ss321(1000\cdot K)}{0.003\cdot in}}}$$

Overall local heat transfer coefficient for the recuperator (assuming gas phase conductivities are about the same

$$hrecavgwc(T) := \frac{1}{\left[\dfrac{1}{\dfrac{\lambda mix(0.01,T)}{\delta gprecup-\dfrac{2\cdot 0.001\cdot cm}{2.976}}}\right]+\left(\dfrac{1}{\dfrac{\lambda mix(0.01,T)}{\delta gprecup}}\right)+\dfrac{1}{\left(\dfrac{\lambda ss321(1000\cdot K)}{0.003\cdot in}\right)}+\dfrac{1}{\dfrac{\lambda wc(0.01,T)}{0.001\cdot cm}}}$$

Effect of wash coat on heat transfer doefficient

$$hrecavg(1000\cdot K)=0.01038\cdot\frac{W}{cm^2\cdot K} \qquad hrecavgwc(1000\cdot K)=0.01046\cdot\frac{W}{cm^2\cdot K}$$

The wash coat makes about 0.1% increase in heat transfer coefficient because of the slightly decreased cell size and greater thermal conductivity of the washcoat vs. gas phase.

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